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(54) Title: MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

#### (57) Abstract

Three-dimensional crystal structure(s) of deacetoxycephalosporin C synthase (DAOCS) are described. The X-ray co-ordinates provide precise 3-dimensional information of amino acids within the structure of DAOCS. Some of these are in complexes with iron and/or substrates. Information from the structures is used to modify enzymes of the cephalosporin biosynthesis pathway including DAOCS, deacetylcephalosporin C synthase DAOC/DACS, such that they accept unnatural substrates (e.g. penicillins G, V) in order to improve the production of beta-lactam antibiotics. The structures may be used to predict the structures of other 2-oxoglutarate dependent enzymes, thereby allowing the design of inhibitors, and new catalysts for the production of e.g. oxidised amino acids/peptides. Specific modifications of amino acid residues are proposed and exemplified.

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وخد

## MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

- Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):
- 1. Conversion of the tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
- In some organisms (e.g. Penicillium chrysogenum and
   Aspergillus nidulans) isopenicillin N is converted by exchange of its <u>L</u>-δ-α-aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced via fermentation under the appropriate conditions.
  - In other organisms (e.g. Streptomyces clavuligerus and Cephalosporium acremonium) isopenicillin N is epimerised to penicillin N.
- This reaction is catalysed by an epimerase enzyme.

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In some organisms (e.g. S. clavuligerus and C. acremonium) 4. penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).

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In some organisms (e.g. S. clavuligerus and C. acremonium) 5. DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. S. clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in C. acremonium DAC may be converted to cephalosporin C and in Streptomyces spp. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, e.g. Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are members of an extended family of Fe(II) utilising oxidase and oxygenase 25 enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS) utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS). Since IPNS, does not use 2-oxoglutarate, it has a substantially different mechanism to the 2-oxoglutarate dependent oxygenases, and this gives 30

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rise to a significantly different active site.

### The Invention

This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes. Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens, Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the beta-barrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach et al., Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. 3-β-hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

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In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the  $\beta$ -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the  $\alpha$ -aminoadipate side chain of the natural substrate and should be changed to a residue of more. hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
  - d) Glu-156. This residue binds with the  $\alpha$ -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- 25 e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
- f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

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Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

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In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

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Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis). However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

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Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus*: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β-hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β-lactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

The iron-free form of DAOCS crystallises in space group R3

as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

### LEGENDS TO FIGURES.

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Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

	Met	Asp	Thr	Thr	Val	Pro	Thr	Phe	Ser	Leu	10
	Ala	Glu	Leu	Gln	Gln	Gly	Leu	His	Gln	Asp	20
	Glu	Phe	Arg	Arg	Cys	Leu	Arg	Asp	Lys	Gly	30
	Leu	Phe	Tyr	Leu	Thr	Asp	Cys	Gly	Leu	Thr	40
5	Asp	Thr	Glu	Leu	Lys	Ser	Ala	Lys	Asp	Leu	50
	Val	Ile	Asp	Phe	Phe	Glu	His	Gly	Ser	Glu	60
•	Ala	Glu	Lys	Arg	Ala	Val	Thr	Ser	Pro	Val	70
	Pro	Thr	Met	Arg	Arg	Gly	Phe	Thr	Gly	Leu	80
	Glu	Ser	Glu	Ser	Thr	Ala	Gln	Ile	Thr	Asn	90
10	Thr	Gly	Ser	Tyr	Ser	Asp	Tyr	Ser	Met	Cys	100
	Tyr	Ser	Met	Gly	Thr	Ala	Asp	Asn	Leu	Phe	110
	Pro	Ser	Gly	Asp	Phe	Gly	Arg	Ile	Trp	Thr	120
•	Gln	Tyr	Phe	Asp	Arg	Gln	Tyr	Thr	Ala	Ser	130
	Arg	Ala	Val	Ala	Arg	Glu	Val	Leu	Arg	Ala	140
15	Thr	Gly	Thr	Glu	Pro	Asp	Gly	Gly	Val	Glu	150
	Ala	Phe	Leu	Asp	Cys	Glu	Pro	Leu	Leu	Arg	160
	Phe	Arg	Tyr	Phe	Pro	Gln	Val	Pro	Glu	His	170
	Arg	Ser	Ala	Glu	Glu	Gln	Pro	Leu	Arg	Met	180
	Ala	Pro	His	Tyr	Asp	Leu	Ser	Met	Val	Thr	190
20	Leu	Ile	Gln	Gln	Thr	Pro	Cys	Ala	Asn	Gly	200
	Phe	Val	Ser	Leu	Gln	Ala	Glu	Val	Gly	Gly	210
	Ala	Phe	Thr	Asp	Leu	Pro	Tyr	Arg	Pro	Asp	220
	Ala	Val	Leu	Val	Phe	Cys	Gly	Ala	Ile	Ala	230
	Thr	Leu	Val	Thr	Gly	Gly	Gln	Val	Lys	Ala	240
25	Pro	Arg	His	His	Val	Ala	Ala	Pro	Arg	Arg	250
	Asp	Gln	Ile	Ala	Gly	Ser	Ser	Arg	Thr	Ser	260
	Ser	Val	Phe	Phe	Leu	Arg	Pro	Asn	Ala	Asp	270
	Phe	Thr	Phe	Ser	Val	Pro	Leu	Ala	Arg	Glu	280
	Cys	Gly	Phe	Asp	Val	Ser	Leu	Asp	Gly	Glu	290
30	Thr	Ala	Thr	Phe	Gln	Asp	Trp	Ile	Gly	Gly	300
	Asn	Tyr	Val	Asn	Ile	Arg	Arg	Thr	Ser	Lys	310
	Ala										311

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# STRUCTURE A

CRYST1	106.400	106.400	71.100	90.00	90.00	120.00
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SCALE3	0.000	0000	0.000000	0.014065	0.0000	00

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                                           55.135 0.542 27.10
ANISOU 8
             CE
                 AMET 1
                           5030
                                   2111
                                           3155
                                                   2345
                                                         -1467 - 9
ATOM
        9
                          30.592
                 AASP 2
             Ν
                                   14.105
                                           59.425 0.268 30.20
                 AASP 2
ANISOU 9
                          4674
             M
                                   3022
                                                   -1210 -782 -383
                                           3777
ATOM
        10
                          29.993
             CA
                 AASP 2
                                   15.322
                                           59.963 0.268 34.22
ANISOU 10
                 AASP 2
             CA
                          5567
                                   2803
                                                   -1106 -964 -525
                                           4633
ATOM
       11
             C
                 AASP 2
                          28.494
                                   15.268
                                           59.655 0.268 33.34
ANISOU 11
                 AASP 2
             C
                          5665
                                   1997
                                           5006
                                                   -314
                                                         -1457 877
ATOM
        12
                 AASP 2
             0
                          28.099
                                   15.650
                                           58.551 0.268 44.76
ANISOU 12
                 AASP 2
             0
                                   5248
                          6859
                                            4901
                                                   -1023 -1582 1631
ATOM
       13
                 AASP 2
             CB
                          30.629
                                   16.528
                                           59.281 0.268 25.98
ANISOU 13
                 AASP 2
             CB
                          4424
                                   3085
                                           2361
                                                   322
                                                         -1794 582
ATOM
             CG
       14
                 AASP 2
                          29.978
                                           59.553 0.268 38.05
                                   17.862
                         <sub>3</sub>6456
ANISOU 14
                AASP 2
             CG
                                   2611
                                           5389
                                                   -501
                                                         -608 -1114
            OD1 AASP 2
ATOM
       15
                          28.995
                                           60.318 0.268 42.35
                                   17.937
            OD1 AASP 2
ANISOU 15
                                   504 9179
                          6406
                                                873
                                                      920 1991
            OD2 AASP 2
ATOM
       16
                          30.449
                                           58.997 0.268 28.59
                                   18.885
ANISOU 16
            OD2 AASP 2
                          1619
                                   2901
                                           6341
                                                   790
                                                         -1022 - 253
ATOM
       17
                 BMET 1
                                   12.640
             Ν
                          32.709
                                           58.544 0.458 29.49
ANISOU 17
             N
                 BMET 1
                          4552
                                                   -105
                                   2218
                                           4435
                                                         1580 477
       18
ATOM
             CA
                 BMET 1
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                                   13.050
                                           57.425 0.458 40.62
ANISOU 18
             CA
                 BMET 1
                          4228
                                           6395
                                   4809:
                                                   580
                                                         210 103
                 BMET 1
ATOM
             C
       19
                          30.884
                                   14.113
                                           57,894 0.458 38.21
ANISOU 19
             C
                 BMET 1
                                           5797
                          5082
                                   3637
                                                   282
                                                         -909 - 915
ATOM
       20
                          30.075
             0
                 BMET 1
                                   14.599
                                           57.110 0.458 44.81
ANISOU 20
             0
                 BMET 1
                          8292
                                   3208
                                           5525
                                                   2071
                                                         -656 - 12
ATOM
       21
             CB
                 BMET 1
                           31.131
                                  11.857 56.829 0.458 33.14
ANISOU 21
             CB
                BMET 1
                          4866
                                   2613
                                           5114
                                                   2013
                                                         -122 8 1 8
       22
ATOM
             CG
                BMET 1
                          29.625
                                           56.968 0.458 40.28
                                   11.840
ANISOU 22
             CG
                BMET 1
                          4795
                                           4768
                                   5740
                                                   230
                                                         -75153
ATOM
       23
                BMET 1
             SD
                          28.761
                                           55.422 0.458 34.23
                                   11.495
ANISOU 23
                BMET 1
             SD
                          5619
                                   3819
                                           3566
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                                                         -215 2 0
ATOM
                BMET 1
       24
             CE
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                                           54.222 0.458 54.24
ANISOU 24
             CE
                BMET 1
                          10672
                                   4519
                                           5420
                                                   1149
                                                         4083 - 2463
ATOM
       25
                 BASP 2
             N
                          30.914
                                           59.194 0.732 37.72
                                   14.381
ANISOU 25
             N
                 BASP 2
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                                   3914
                                                   -1323 -1208 -1385
ATOM
       26
                BASP 2
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                                           59.811 0.732 35.78
ANISOU 26
                 BASP 2
             CA
                          5412
                                   3387
                                           4794
                                                   -1064 -1050 - 795.
ATOM
       27
             C
                 BASP 2
                          28.536
                                   14.886
                                           59.567 0.732 29.66
ANISOU 27
             C
                 BASP 2
                          4876
                                   1624
                                            4771
                                                   27 -1561 1218
ATOM
       28
                 BASP 2
             0
                          28.181
                                           58.414 0.732 34.65
                                   14.602
ANISOU 28
                 BASP 2
             0
                          4375
                                   3689
                                           5100
                                                   65 -1485 2 4 7
ATOM
       29
                BASP 2
             CB
                           30.195
                                   16.696
                                           59.181 0.732 37.39
ANISOU 29
                BASP 2
             CB
                           6632
                                   3351
                                            4222
                                                   -1850 869 -1518
ATOM
       30
             CG
                 BASP 2
                           29.562
                                           60.104 0.732 30.38
                                   17.730
ANISOU 30
            CG BASP 2
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                                                   -500 -606 -1191
                                   3791
                                            4510
MOTA
             OD1 BASP 2
        31
                           28.866
                                   17.247
                                           61.030 0.732 48.88
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- 14 -ANISOU 31 OD1 BASP 2 4203 6276 8095 -1203 3147 -1901 ATOM 32 OD2 BASP 2 29.760 59.875 0.732 34.85 18.945 ANISOU 32 OD2 BASP 2 2852 3708 6680 -491 444 - 1450ATOM 33 THR N 27.717 3 14.789 60.606 1.000 35.58 ANISOU 33 4123 N THR 3 4586 4811 601 -1628 1516 ATOM CA34 THR 60.495 1.000 40.48 3 26.303 14.433 ANISOU 34 CA THR 3 4650 4555 6175 371 -911 - 385ATOM 35 C 3 THR 25.382 60.611 1.000 39.82 15.647 ANISOU 35 C THR 3 4376 4155 6598 320 -3864 -586 ATOM 36 0 THR 3 24.150 60.751 1.000 33.55 15.556 ANISOU 36 0 THR 3 4668 3107 4972 -2748 -588 357 ATOM 37 CB 25.905 THR 3 13.450 61.613 1.000 39.95 ANISOU 37 CB THR 3787 3 4004 7387 160 -1209 6 2 OG1 THR ATOM 38 3 26.591 62.817 1.000 61.83 13.851 ANISOU 38 OG1 THR 5882 10134 -4164 -3020 2051 7476 CG2 THR 39 ATOM 26.399 12.052 3 61.278 1.000 59.32 CG2 THR ANISOU 39 3 4613 3971 13955 1114 -3135 - 198ATOM 40 NTHR 4 16.780 26.036 60.456 1.000 32.55 ANISOU 40 N THR 4 4306 4611 3450 377 -2166 - 217ATOM 41 ·CA THR 25.439 4 60.393 1.000 31.22 18.092 ANISOU 41 CATHR 4275 4 4229 3358 -81 -1179 9 5 42 ATOM C THR 24.672 59.090 1.000 30.06 4 18.272 C ANISOU 42 THR 4 4876 3341 3207 773 -1156 - 204ATOM 43 THR 0 25.195 58.017 1.000 31.64 4 17.935 ANISOU 43 THR 4 4877 3780 3363 1935 -1255 - 52ATOM 44 CB THR 4 26.510 19.208 60.407 1.000 32.31 ANISOU 44 CB THR 4 2320 4762 5194 475 -547593OG1 THR ATOM 45 27.324 4 19.091 61.578 1.000 32.36 ANISOU 45 OG1 THR 4 3705 3955 4635 -797 - 389-79 CG2 THR ATOM 46 25.852 4 20.582 60.458 1.000 27.22 ANISOU 46 CG2 THR 3728 4 4174 2443 71 304 - 151 ATOM 47 VAL N 5 23.464 59.211 1.000 21.69 18.796 ANISOU 47  $\mathbf{N}$ VAL 5 4041 1985 2215 -543 -657 1 5 8 ATOM 48 ÇA VAL 5 22.690 58.024 1.000 20.42 19.140 ANISOU 48 VAL CA5 3675 1964 2120 -517 1 0 3 -622 VAL ATOM 49 C 5 23.199 57.499 1.000 17.01 20.489 ANISOU 49 C VAL 5 2263 1803 2396 -279 -622 8 9 50 ATOM 23:156 VAL 0 21.449 58.252 1.000 21.10 ANISOU 50 5 1885 VAL 3662 -389 2472 -656 1 6 ATOM 51 CB VAL 21.204 58.402 1.000 24.22 19.216 ANISOU 51 CB VAL 3551 2155 3495 -1045 -396 7 8 3 52 ATOM CG1 VAL 5 20.434 19.700 57.166 1.000 20.14 CG1 VAL ANISOU 52 3202 -453 10 -226 1779 2672 ATOM 53 CG2 VAL 20.701 58.860 1.000 28.58 17.867 ANISOU 53 CG2 VAL 5258 2086 3516 -1226 431 5 1 0 ATOM 54 PRO 23.750 20.542 N 56.300 1.000 16.95 ANISOU 54 PRO N 2378 1629 2434 29 -594 301 ATOM 55 24.354 21.793 CA PRO 6 55.857 1.000 16.90 ANISOU 55 PRO CA 1645 1775 3000 6 - 445 303ATOM 56 C PRO 6 23.298 22.800 55.383 1.000 15.61 ANISOU 56 C PRO 1477 1766 2687 -192 -437 5 4 5 ATOM 57 PRO 0 6 22.133 22.432 55.201 1.000 15.75 ANISOU 57 PRO 1578 0 1761 2647 -260 -579 5 5 ATOM 58 CB PRO 25.216 54.682 1.000 19.85 21.375 ANISOU 58 CB PRO 2320 1752 3468 50 70 182 ATOM 59 CG PRO 24.632 20.095 54.187 1.000 24.76 ANISOU 59 CG PRO 6 3550 2953 2904 -1186300-286ATOM 60 CD PRO 23.926 55.357 1.000 17.91 19.428 ANISOU 60 CD PRO 1960 1962 2882 -168 -138 - 44 ATOM 61 THR N 23.723 24.031 55.156 1.000 14.38 ANISOU 61 THR N 1518 1567 2378 -158 -616 1 0 0

- 15 -ATOM 62 CA THR 22.907 7 25.103 54.610 1.000 14.09 ANISOU 62 THR CA1625 7 1554 2174 -255 -581 2 2 8 ATOM 63 C THR 7 23.605 25.684 53.374 1.000 14.74 ANISOU 63 C THR 7 1683 1849 2067 -193 -468 1 2 1 ATOM 64 THR 7 0 24.828 25.894 53.423 1.000 15.95 ANISOU 64 THR 0 7 1752 2137 2171 -378 -457 1 8 5 ATOM 65 22.795 CB THR 7 26.248 55.637 1.000 15.25 CB ANISOU 65 THR 7 1548 1846 56 -124 2401 OG1 THR ATOM · 66 7 22.208 25.717 56.829 1.000 16.91 ANISOU 66 OG1 THR 7 1818 2149 2458 -402 -18347CG2 THR ATOM 67 7 27.387 21.952 55.040 1.000 16.09 CG2 THR ANISOU 67 7 1613 1651 2848 -138 -263 - 25ATOM 68 PHE N 8 22.830 25.892 52.325 1.000 15.06 ANISOU 68 PHE N 8 1618 1966 2137 -558 2 3 0 -411ATOM 69 PHE CA8 23.317 26.545 51.136 1.000 14.76 ANISOU 69 PHE ÇA 8 1558 1857 2192 -213-411 2 8 1 ATOM 70 C PHE 8 22.421 50.810 1.000 14.94 27.728 ANISOU 70 C PHE 8 1907 1421 2347 -275 -357 1 8 1 ATOM 71 PHE 0 8 21.198 27.678 50.995 1.000 16.40 ANISOU 71 0 PHE 8 1782 1642 2808 -197 -550 3 4 72 ATOM PHE CB 8 23.242 25.562 49.948 1.000 16.49 ANISOU 72 CB PHE 8 2123 1854 49 - 371 - 1 2287 73 ATOM CGPHE 8 24.225 24.432 50.027 1.000 14.92 ANISOU 73 PHE CG 8 1710 1824 2135 -197 -365 1 6 3 ATOM CD1 PHE 74 8 23.822 23.227 50.600 1.000 16.78 CD1 PHE ANISOU 74 1808 8 1726 2842 -300 -358 1 8 4 CD2 PHE 75 ATOM 8 25.539 24.558 49.602 1.000 16.67 ANISOU 75 CD2 PHE 2130 8 1705 2500 -310 -361 3 2 1 ATOM 76 CE1 PHE 24.702 8 22.183 50.742 1.000 16.74 CE1 PHE ANISOU 76 8 2035 1966 -4 -99 2 9 5 2359 CE2 PHE ATOM 77 8 26.420 49.773 1.000 19.18 23.525 ANISOU 77 CE2 PHE 8 1398 2153 3736 -408 -631 1 8 7 ATOM 78 CZPHE 22.336 8 26.026 50.351 1.000 17.90 ANISOU 78 CZPHE 8 1849 2948 2003 -119-376 2 0 ATOM 79 N SER 9 23.023 28.776 50.314 1.000 14.82 ANISOU 79 NSER 9 2134 1488. 2008 -351 -528 3 1 0 ATOM 80 CASER 9 22.338 49.715 1.000 15.12 29.902 ANISOU 80 SER CA9 2037 1259 2449 -357 -571 1 3 4 ATOM 81 C SER 9 21.977 29.607 48.270 1.000 16.19 ANISOU 81 C SER 9 2138 1791 2224 -374 -535 5 4 7 ATOM 82 SER 9 22.877 47.473 1.000 17.04 29.312 ANISOU 82 0 SER 9 2191 1892 2393 -423 -544 2 3 2 ATOM 83 SER 23.306 CB 9 31.113 49.696 1.000 18.74 ANISOU 83 SER CB 9 2891 1712 2519 -1012 -478 7 1 7 ATOM SER 84 OG 9 22.738 32.131 48.853 1.000 20.82 ANISOU 84 9 SER OG 2866 1569 -662 -854 6 0 7 3477 ATOM 85 LEU  $\mathbf{N}$ 10 20.697 47.924 1.000 16.46 29.674 ANISOU 85 LEU N 2215 10 1495 2542 -228 -740 -48ATOM 86 LEU CA20.345 29.401 10 46.529 1.000 17.55 ANISOU 86 LEU CA10 2263 1856 2551 -582 -694 3 6 ATOM 87 C LEU 21.079 10 45.591 1.000 18.84 30.373 ANISOU 87 C LEU 2506 10 1870 2784 -596 -830 3 5 7 ATOM 88 LEU 0 10 21.573 30.025 44.520 1.000 20.19 ANISOU 88 LEU 0 10 2705 2263 2704 -524 -663 5 0 8 ATOM 89 LEU CB 10 18.844 29.559 46.327 1.000 18.87 ANISOU 89 CB LEU 2302 10 2516 -288 -715 2 8 0 2354 ATOM 90 CG LEU 18.355 10 44.895 1.000 18.28 29.333 ANISOU 90 LEU CG 2182 10 2172 -668 -677 - 301 2591 ATOM 91 CD1 LEU 18.708 10 27.955 44.397 1.000 22.45 ANISOU 91 CD1 LEU 3418 10 2024 3089 -308 -537 1 7 ATOM 92 CD2 LEU 16.852 10 29.603 44.869 1.000 21.93

		- 16 -		
ANISOU 92 ATOM 93 ANISOU 94 ANISOU 94 ANISOU 95 ANISOU 96 ANISOU 97 ANISOU 97 ANISOU 97 ANISOU 99 ANISOU 100 ATOM 101 ANISOU 101 ANISOU 102 ANISOU 102 ANISOU 103 ANISOU 103 ANISOU 103 ANISOU 104 ANISOU 105 ANISOU 106 ANISOU 106 ANISOU 106 ANISOU 107 ANISOU 108 ANISOU 108 ANISOU 109 ANISOU 111 ANISOU 113 ANISOU 113 ANISOU 113 ANISOU 113 ANISOU 113 ANISOU 115 ANISOU 117 ANISOU 117 ANISOU 117 ANISOU 118 ANISOU 118 ANISOU 119 ANISOU 119 ANISOU 119 ANISOU 1118 ANI	C GLU 12 O GLU 12 O GLU 12 C G GLU 12 C G GLU 12 C G GLU 12 C C G GLU 12 C C C C C C C C C C C C C C C C C C C	-16- 2250	2977 -595 45.202 1.000 4380 -455 44.946 1.000 2937 -644 43.829 1.000 3158 -1628 45.953 1.000 3044 -828 45.862 1.000 2615 -506 44.920 1.000 2117 -702 44.069 1.000 2117 -702 44.069 1.000 2117 -1148 47.204 1.000 2636 -221 48.032 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 3169 -1297 49.803 1.000 3169 -1348 50.092 1.000 3888 -1119 42.738 1.000 2275 -351 44.174 1.000 2275 -351 44.174 1.000 2275 -351 44.174 1.000 2149 -209 42.738 1.000 2149 -209 41.824 1.000 2149 -209 42.738 1.000 2149 -209 41.824 1.000 2149 -209 42.738 1.000 2149 -209 41.824 1.000 2149 -209 42.738 1.000 2149 -209 41.824 1.000 41.824 1.000 41.824 1.000 41.824 1.000 41.824 1.000 41.824 1.000 41.824 1.000 41.824	0 2 0 . 0 5 -1279 4 7 2 0 2 4 . 2 4 -979 8 9 1 0 2 1 . 0 6 -1016 4 3 1 0 2 6 . 2 9 3 -923 1 1 3 7 0 2 4 . 2 9 -216 9 9 6 2 0 . 6 5 -930 6 7 4 2 1 . 1 9 -715 5 9 8 2 1 . 5 6 2 2 1 . 9 8 1 - 488 6 1 8 2 0 . 2 7 -624 5 0 1 2 0 . 5 4 -516 4 0 6 2 1 . 8 6 9 2 4 . 9 8 1 - 20 6 9 8 8 2 1 . 8 6 1 2 0 . 5 4 6 2 1 . 8 6 9 2 4 . 9 8 1 3 3 . 5 2 1 8 . 6 1 2 7 0 4 0 6 2 1 . 4 0 -4 1 5 2 6 2 3 . 7 5 -1 1 7 1 9 0 1 8 . 9 7 -1 4 5 4 4 0 1 8 . 5 7 -1 4 5 9 4 1 9 . 8 0 -1 4 2 5 9 4 1 9 . 8 0 -2 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 7 4 -1 4 2 5 9 4 1 9 . 8 0 -3 0 . 0 4 -4 2 7 8 9 8 2 6 . 2 8
ANISOU 118 ATOM 119	O GLN·14 CB GLN 14	3836 4657 22.064 30.906 3133 3630 20.772 30.111 3106 2319 19.586 31.020 3384 2462	2922 -1208 41.131 1.000 3222 -760 41.355 1.000 3413 -299 41.631 1.000 3155 -317	-427 8 9 8 26.28 -863 9 3 8 23.26 -577 5 1 4 23.69 -393 - 1 9 6
ANISOU 122	OE1 GLN 14	19.734 32.104 4973 2619	42.160 1.000 3175 -183	

**,** -5

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- 17 -ATOM 123 NE2 GLN 14 18.398 30.513 41.349 1.000 23.60 ANISOU 123 NE2 GLN 3058 14 2969 2941 -383 54 2 4 5 ATOM 124 GLN 25.309 N 15 31.243 41.395 1.000 25.00 ANISOU 124 15 GLN N 3078 3281 3140 -1159 -394 5 7 5 ATOM 125 CA15 GLN 26.530 31.936 40.945 1.000 24.05 ANISOU 125 CA 15 2947 3560 GLN 2631 -866 5 5 5 -98 ATOM 126 C GLN 15 27.650 30.920 40.707 1.000 26.06 ANISOU 126 GLN C 15 .3810 3951 2139 -345406 668 127 ATOM 0 15 GLN 28.756 40.302 1.000 35.85 31.284 ANISOU 127 GLN 15 0 4294 4851 4476 1871 1192 102 ATOM 15 128 GLN CB 27.018 32.918 42.009 1.000 25.90 ANISOU 128 15 CB GLN 3055 3037 3748 -1092 -109 3 6 4 ATOM 129 CG GLN 15 26.103 34.092 42.219 1.000 31.24 ANISOU 129 CG 15 GLN 4562 2577 4731 -806 962 1054 ATOM 130 GLN CD15 35.022 26.503 43.348 1.000 59.75 ANISOU 130 CDGLN 15 9927 2475 -1855 -14 -1904 10301 131 ATOM OE1 GLN 15 27.634 35.031 43.840 1.000 81.81 ANISOU 131 15 OE1 GLN 15059 3931 12094 -944 -6272 - 1803ATOM 132 NE2 GLN 25.539 15 35.841 43.767 1.000 91.46 NE2 GLN ANISOU 132 15 14070 4846 15833 -923 3672 - 4850 ATOM 133 N GLY 16 27.379 29.643 40.969 1.000 29.90 ANISOU 133 N GLY 4634 16 3820 2907 -239 22 7 8 7 ATOM 134 CAGLY 16 28.410 28.649 40.699 1.000 28.76 ANISOU 134 GLY 3629 CA16 4466 2833 -709 2 5 0 461 ATOM 135 C GLY 16 28.473 29.339 41.878 1.000 27.60 ANISOU 135 GLY 3779 C 3816 16 2891 -616 914 1485 ATOM 136 GLY 0 16 27.867 30.398 41.725 1.000 31.47 ANISOU 136 GLY 0 16 3386 4758 3814 -899 1243 1023 137 ATOM N LEU 17 28.960 28.898 43.083 1.000 26.01 ANISOU 137 N LEU 3295 17 3636 2950 -721 162 7 4 3 138 ATOM CA17 LEU 29.776 44.257 1.000 23.96 28.666 ANISOU 138 CA 2700 17 LEU 3032 3372 -601 100 673 ATOM 139 C LEU 17 29.462 27.338 44.932 1.000 20.31 ANISOU 139 C LEU 17 2222 2763 2733 -252 611 261 ATOM 140 LEU 28.389 0 17 26.780 44.789 1.000 23.13 ANISOU 140 0 LEU 17 2347 3308 3134 -443 263 8 5 9 ATOM 141 CB LEU 17 29.645 45.286 1.000 25.94 29.806 ANISOU 141 CB LEU 2933 2886 17 -1318 -405 2 5 4 4035 ATOM 142 CG LEU 17 29.962 31.209 44.716 1.000 31.57 ANISOU 142 CG 17 2948 LEU 3741 5308 -523 1150 7 2 2 ATOM 143 CD1 LEU 45.615 1.000 32.04 17 29.550 32.358 CD1 LEU 5221 ANISOU 143 17 2887 4066 -1269 278 508 ATOM 144 CD2 LEU 17 31.458 31.278 44.416 1.000 38.11 CD2 LEU ANISOU 144 3828 17 5491 -2315 954 232 5160 MOTA 145 N HIS 18 30.441 45.681 1.000 22.49 26.822 ANISOU 145 2600 HIS N 18 3067 2877 -662 42 4 4 9 ATOM 146 HIS CA30.289 18 25.644 46.537 1.000 21.54 ANISOU 146 CAHIS 2378 2809 18 -432 201 313 2996 ATOM 147 C HIS 29.908 18 24.376 45.790 1.000 22.76 ANISOU 147 C HIS 18 2256 3245 3148 -1009 282 114 ATOM 148 HIS 0 18 29.147 23.565 46.331 1.000 22.60 ANISOU 148 HIS 18 2008 3064 3516 -629 -166 8 8 4 MOTA 149 CB HIS 29.224 25.872 18 47.618 1.000 22.81 ANISOU 149 HIS CB 18 2514 -526 450 421 2879 3272 ATOM 150 HIS CG 18 29.320 48.217 1.000 21.70 27.248 ANISOU 150 CG HIS 2797 18 3038 -149 39 5 0 3 2411 151. ATOM ND1 HIS 18 30.438 48.807 1.000 25.01 27.773 ANISOU 151 ND1 HIS 3714 18 3505 2284 -207 -629 1 4 9 ATOM 152 CD2 HIS 18 28.370 28.216 48.269 1.000 24.95 ANISOU 152 CD2 HIS 3244 18 3278 2957 87 544 2 7 5 CE1 HIS MOTA 153 30.197 28.982 18 49.223 1.000 29.26

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- 18 -
 ANISOU 153
              CE1 HIS
                        18
                            4603
                                    3396
                                            3118
                                                          -335 2 7
                                                    -388
 ATOM
         154
              NE2 HIS
                           28.937
                        18
                                    29.271
                                            48.919 1.000 27.24
 ANISOU 154
              NE2 HIS
                        18
                           4582
                                    3137
                                            2632
                                                       224 3 6 5
                                                    2
 ATOM
         155
              M
                  GLN
                           30.269
                        19
                                    24.270
                                            44.521 1.000 22.74
 ANISOU 155
              N
                  GLN
                           2724
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                                            2822
                                                    -511
                                                          -123 4 2 3
 ATOM
         156
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                       19
                                    23.113
                                            43.730 1.000 23.85
 ANISOU 156
              CA
                  GLN
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                       19
                                    2668
                                            3263
                                                    148
                                                          63 8 9
 ATOM
         157
              C
                  GLN
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                       19
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                                            44.221 1.000 22.77
 ANISOU 157
                  GLN
                           2532
                       19
                                    3026
                                            3095
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                                                          -574 7 7 8
 ATOM
         158
              0
                  GLN
                       19
                           29.480
                                    20.801
                                            44.259 1.000 21.99
 ANISOU 158
              0
                  GLN
                       19
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                                    2911
                                            3574
                                                   -187
 ATOM
        159
              CB
                  GLN
                       19
                                   23.322
                           30.227
                                            42.276 1.000 27.66
 ANISOU 159
              CB
                  GLN
                       19
                                   2519
                           5043
                                            2947
                                                   29 -339 458
 ATOM
        160
              CG
                  GLN
                       19
                           29.397
                                   24.333
                                            41.523 1.000 26.21
 ANISOU 160
              CG
                  GLN
                       19
                           3289
                                    3163
                                            3508
                                                   299
                                                          171 4 3 7
 ATOM
        161
                  GLN
              CD
                           27.917
                       19
                                   24.368
                                            41.862 1.000 32.47
 ANISOU 161
                 GLN
              CD
                       19
                           3403
                                   4411
                                            4521
                                                   -986
                                                        535 654
 ATOM
             OE1 GLN
        162
                       19
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                                   6893
                                           5705
                                                        1323 - 1915
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ATOM
        170
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                                                         1508 - 797
ATOM
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                                   20.433
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                                   8705
                                           6277
                                                   -589 1088 - 87
ATOM
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                                   21.053
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ATOM
       180
            OE2 GLU
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ANISOU 180
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- 19 -MOTA 184 PHE 0 22 25.867 18.574 46.995 1.000 15.87 ANISOU 184 PHE 22 0 1570 2118 2343 -249 -361 1 3 1 185 ATOM CB 26.305 PHE 22 21.840 46.149 1.000 18.00 ANISOU 185 CB PHE 22 1747 2754 2337 70 -178 4 4 5 MOTA 186 CG PHE 22 24.802 21.729 45.930 1.000 16.38 ANISOU 186 PHE CG 22 1763 1748 2714 -326 2 2 3 -90 MOTA 187 CD1 PHE 22 23.934 21.723 47.003 1.000 18.29 ANISOU 187 CD1 PHE 22 1812 2091 3045 -197 5 7 6 -88 CD2 PHE ATOM 188 22 24.290 21.720 44.641 1.000 18.62 ANISOU 188 2106 CD2 PHE 22 2079 2890 -623 3 9 4 -143ATOM 189 CE1 PHE 22 22.569 21.727 46.771 1.000 18.90 ANISOU 189 CE1 PHE 1826 22 3271 2086 -198 -133 3 0 2 CE2 PHE 190 ATOM 22 22.911 21.660 44.379 1.000 19.28 ANISOU 190 CE2 PHE 22 2189 2023 3114 -242 -754 - 144ATOM 191 CZPHE 22 22.059 21.645 45.473 1.000 19.42 ANISOU 191 CZPHE 2048 22 1723 3607 90 -483 - 376 MOTA 192 N ARG 23 27.580 45.583 1.000 17.88 18.971 ANISOU 192 N ARG 23 1647 2437 2709 -168 -218317ATOM 193 CAARG 23 27.520 17.594 45.079 1.000 19.18 ANISOU 193 CAARG 23 1724 2539 3022 36 158 -166 ATOM 194 C ARG 23 27.767 16.595 46.211 1.000 19.11 ANISOU 194 C ARG 23 1279 2461 3518 -173 -113 4 5 5 ATOM 195 0 ARG 23 27.107 15.547 46.229 1.000 18.82 ANISOU 195 0 ARG 23 1614 2156 3381 -33 -128 181 ATOM 196 CB ARG 23 28.605 17.351 44.030 1.000 22.81 ANISOU 196 CB ARG 23 1934 4099 2633 -34 -105 - 354ATOM 197 CG 23 ARG 17.790 28.248 42.617 1.000 24.82 ANISOU 197 CG ARG 23 2601 4078 2752 191 -122 - 204ATOM 198 CD ARG 23 ~29.376 17.272 41.685 1.000 29.71 ANISOU 198 CDARG 23 5619 2503 -285 3168 908 704 MOTA 199 NE **ARG** 23 30.479 41.800 1.000 30.96 18.206 ANISOU 199 NE ARG 23 2877 5034 3851 -43 286 ATOM 200 CZARG 23 30.549 19.360 41.148 1.000 29.49 ANISOU 200 CZARG 23 2612 5063 3529 -225 606 177 ATOM 201 NH1 ARG 23 29.536 19.665 40.328 1.000 29.26 ANISOU 201 NH1 ARG 23 3242 4951 2923 -960 331 5 2 5 ATOM 202 NH2 ARG 23 31.629 41.345 1.000 32.61 20.092 ANISOU 202 NH2 ARG 23 2320 5347 4722 -134519 179 MOTA 203 N ARG 28.708 24 16.851 47.125 1.000 17.80 ANISOU 203 N ARG 24 1262 3332 2168 38 9 8 183 ATOM 204 CA ARG 24 28.930 15.899 48.222 1.000 18.85 ANISOU 204 CAARG 24 2509 3287 1368 69 -162 105 205 ATOM C ARG 27.701 15.811 24 49.114 1.000 17.51 ANISOU 205 ARG C 1456 24 2015 3181 132 -177243ATOM 206 ARG 24 27.333 14.733 49.544 1.000 17.93 ANISOU 206 ARG 1851 1965 24 2997 -16 -402253ATOM 207 CB ARG 24 30.203 16.321 48.991 1.000 19.88 ANISOU 207 CB ARG 24 1685 2700 3169 -398 -218 4 4 ATOM 208 CG ARG 24 31.459 16.053 48.135 1.000 29.07 ANISOU 208 CG ARG 24 1467 4625 4954 269 203 709 ATOM 209 CD ARG 32.700 24 16.206 49.016 1.000 41.84 ANISOU 209 CD ARG 24 1745 7021 7130 -451 -494 -922 ATOM 210 ARG ΝE 24 33.690 17.103 48.464 1.000 57.06 ANISOU 210 NE 4362 ARG 24 9316 8003 -3326 -669 -1141 ATOM 211 CZARG 24 34.032 18.327 48.810 1.000 60.67 ANISOU 211 CZARG 24 10369 5961 6723 -4627 -1324 -1586 ATOM NH1 ARG 212 24 33.430 18.980 49.799 1.000 49.70 ANISOU 212 NH1 ARG 24 7748 6565 4569 -951 -2185 2226 ATOM 213 NH2 ARG 24 34.997 48.159 1.000 54.12 18.971 ANISOU 213 NH2 ARG 24 8696 3378 -3780 -2352 1607 8490 ATOM 214 CYS N 27.092 16.963 49.370 1.000 15.74 25

								1 C 1/G D / 0/03000
ANISO	U 214	N	CYS	25	1425	- 20 -		
ATOM	215	CA	CYS	25	1435 25.884	1969	2574	-16 -393 - 33
ANISO	J 215	CA		25	1518	16.921 1954	50.223	
ATOM	216	C	CYS	25	24.826	15.068	2756 49.547	-95 $-317$ $-300$ $7$ 1.000 15.73
ANISO		C	CYS	25	1629	1699	2648	
ATOM	217	0	CYS	25	24.124	15.262		-114 -432 6 6 5 1.000 15.89
ANISO		0	CYS	25	1453	1801	2783	-88 -469 2 5 2
ATOM ANISOU	218 J 218	CB CB	CYS	25	25.367	18.362	50.424	
ATOM	219	SG	CYS CYS	25 25	1644	1779	2629	-49 -261 - 30
ANISOU		SG.	CYS		23.700 1742	18.417	51.184	
ATOM	220	N	LEU	26	24.623	1825 16.308	3202	-122 -33 -55
ANISOU		N	LEU	26	1449	1843	48.250 2504	
ATOM	221	CA	LEU	26	23.560	15.590	47.534	
ANISOU ATOM	221	CA	LEU	26	1616	1739	2580	-86 -453 4 8
ANISOU		C C	LEU LEU	26	23.763	14.085	47.621	
ATOM	223	0	LEU	26 26	1697	1764	2306	-113 -479 6
ANISOU		Ö	LEU	26	22.819 1797	13.345 1725	47.771	
ATOM	224	CB	LEU	26	23.526	16.068	2920 46.066	-234 -664 -300
ANISOU		CB	LEU	26	1811	1645	2633	1.000 16.02 -191 -483 122
ATOM	225	CG	LEU	26	23.057	17.510	45.864	
ANISOU ATOM	225 226	CG CD1	LEU	26	1762	1716	2485	-6 -15 7 9
ANISOU			LEU LEU	26 26	23.252	17.880	44.405	1.000 17.48
ATOM	227		LEU	26	1750 21.584	2360	2532	-17 -130 4 6 5
ANISOU	227		LEU	26	1655	17.680 2188	46.290 2660	
ATOM	228	N	ARG	27	25.027	13.648	47.494	-29 -75 168 1.000 17.26
ANISOU ATOM	228 229	N	ARG	27	1870	1818	2871	155 -326 1 4 0
ANISOU		CA CA	ARG ARG	27	25.295	12.205	47.372	
ATOM	230	C	ARG	27 27	2108 25.240	1845	3170	270 -955 1 0 2
ANISOU	230	C	ARG	27	1667	11.599 1801	48.744 3351	
ATOM	231	0	ARG	27	24.777	10.454	48.913	159 -897 2 1 9 1.000 2 0 . 9 9
ANISOU	231	0	ARG	27	2158	1793	4026	-43 -360 1 6 8
ATOM ANISOU	232 232	CB	ARG	27	26.641	12.008	46.670	
ATOM	233	CB N	ARG ASP	27 28	2815	2034	3264	622 -377 -129
ANISOU	233	N	ASP	28	25.827 1487	12.293	49.723	
ATOM	234	CA	ASP	28	26.034	2004 11.672	2856 51.026	178 -328 6 7
ANISOU	234	CA	ASP	28	1613	2095	2931	1.000 17.47 107 -301 1 2 7
ATOM ANISOU	235	C	ASP	28	24.872	11.866	51.990	1.000 17.22
ATOM	235 236	C 0	ASP	28	1414	2264	2863	223 -447 4 7 1
ANISOU	236	0	ASP ASP	28 28	24.816	11.081	52.937	
ATOM	237	CB	ASP	28	1932 27.306	2139 12.237	2624	150 -565 3 2 7
ANISOU	237	CB	ASP	28	1581	3894	51.657 2948	
ATOM	238		ASP	28	28.590	11.906		-272 -467559 $1.00024.72$
ANISOU ATOM	238		ASP	28	1596	3323	4472	236 -288 6 4 8
ANISOU	239 239		ASP	28	28.572	10.905	50.199	1.000 27.56
ATOM	240	OD2	ASP	28 28	2317	3071	5084	808 -284 5 7 2
ANISOU	240	OD2		28	29.573 1584	12.617 4343		1.000 32.08
ATOM	241		LYS	29	24.098	12.942	6261	-144 -470 4 1 6
ANISOU	241	N	LYS	29	1475	1814	2627	1.000 15.57 5 -303 178
ATOM ANISOU	242		LYS	29	23.048	13.305		1.000 15.13
ATOM	242 243	_	LYS	29	1584	1999	2165	-68 -500 - 96
ANISOU	243		LYS LYS	29 29	21.686	13.500		1.000 14.56
ATOM	244		LYS	29	1496 20.688	1352 12.985	2686	77 -452 106
ANISOU	244	0	LYS	29	1627	1876	52.635 2657	1.000 16.21 -177 -315 - 5
						_ + , \	2001	-177 -315 - 5

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245
MOTA
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ANISOU 245
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ANISOU 248
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ATOM
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                                           55.039 1.000 20.16
ANISOU 259
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                LEU
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ATOM
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            CD2 LEU
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            CD2 LEU
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ANISOU 267
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ATOM
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            CD2 PHE
ATOM
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ANISOU 270
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            CE2 PHE
MOTA
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ANISOU 271
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MOTA
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ATOM 276	O TYR	33 20.158	24.871 52.85	
ANISOU 276	O TYR	33 1370	1524 2912	-190 -420 2 6 3
ATOM 277 ANISOU 277	CB TYR	33 18.874	24.734 55.85	· · · · · · · · · · · · · · · · · · ·
ATOM 278	CB TYR CG TYR	33 1648	1717 2133	-197 -309 -131
ANISOU 278	CG TYR	33 18.231 33 2131	24.046 57.04	
ATOM 279	CD1 TYR	33 16.938	1537 2302 24.390 57.45	-339 -109 -136
ANISOU 279	CD1 TYR	33 2478	24.390 57.45 1967 2172	
ATOM 280	CD2 TYR	33 18.912	23.116 57.79	
ANISOU 280	CD2 TYR	33 2901	2070 2468	144 115 192
ATOM 281	CE1 TYR	33 16.354	23.758 58.54	
ANISOU 281 ATOM 282	CE1 TYR	33 3138	1948 2581	26 740 - 102
ANISOU 282	CE2 TYR CE2 TYR	33 18.368	22.475 58.90	
ATOM 283	CZ TYR	33 3571 33 17.081	2480 2118	340 196 122
ANISOU 283	CZ TYR	33 4140	22.821 59.26 1772 2454	
ATOM 284	OH TYR	33 16.541	22.194 60.35	471 1035 - 105 5 1.000 29.55
ANISOU 284	OH TYR	33 5088	2809 3329	377 1512 7 2 8
ATOM 285		34 18.076	25.709 52.87	
ANISOU 285		34 1496	1533 2396	-80 -517 - 17
ATOM 286 ANISOU 286		34 18.278	26.620 51.75	6 1.000 15.02
ATOM 287	CA LEU C LEU	34 1830 34 17.871	1452 2425	-126 -580 2 0
ANISOU 287		34 17.871 34 1703	28.039 52.15 1575 2217	= · · · · · · = · · · · · · ·
ATOM 288	_	34 16.716	1575 2217 28.289 52.49	-146 -241 - 7 $2 1.000 16.95$
ANISOU 288		34 1663	1852 2923	2 1.000 16.95 -75 -186 - 64
ATOM 289		34 = 17.389	26.127 50.59	<del>-</del>
ANISOU 289		34 2355	1485 2444	-212 -749 2 5
ATOM 290 ANISOU 290		34 17.633	26.800 49.24	9 1.000 15.65
ATOM 291		34 2010 34 18.977	1567 2371	-7 -633 - 63
ANISOU 291		34 18.977 34 1919	26.422 48.66 2018 3717	
ATOM 292		34 16.490	2018 3717 26.535 48.29	-225 -171 2 6 0 1 1.000 17.29
ANISOU 292		34 2152	1824 2592	-425 -819 2 1 4
ATOM 293		35 18.842	28.944 52.06	
ANISOU 293		35 1817	1532 2534	-230 -200 1 3
ATOM 294 ANISOU 294	_	35 18.587	30.362 52.32	
ATOM 295		35 2149 35 18.491	1537 2781	-206 -827 -196
ANISOU 295		35 18.491 35 1895	31.127 51.01 1693 2887	
ATOM 296		35 18.765	1693 2887 30.572 49.93	-149 -882 - 4 4 8 1.000 17.01
ANISOU 296		35 1880	1692 2893	8 1.000 17.01 -262 -458 1 4 4
ATOM 297		35 19.772	30.917 53.18	
ANISOU 297		35 2018	1942 2800	-87  -854  -200
ATOM 298 ANISOU 298		35 20.986	30.673 52.47	
ATOM 299		35 2110 35 19.847	2035 3873	-253 -364 - 402
ANISOU 299		35 19.847 35 2600		7 1.000 20.44
ATOM 300		36 18.186	2194 2971 32.407 51.05	228 -1113 5 9 9 1.000 18.62
ANISOU 300		36 2287	1747 3040	· · · · · · · · · · · · · · · · · · ·
ATOM 301	CA ASP	36 18.240	33.300 49.88	
ANISOU 301	_	36 2678	1722 3483	-632 -508 3 7 4
ATOM 302 ANISOU 302		36 17.474		3 1.000 20.05
ATOM 303		36 2104 36 17.929	1929 3586	
ANISOU 303	-	36 17.929 36 2593	32.685 47.54 1749 3662	
ATOM 304		36 19.703	1749 3662 33.561 49.50	-496 -756 1 3 1 0 1.000 22.21
ANISOU 304		36 2666	2366 3406	-876 -755 8 0 7
ATOM 305	CG ASP	36 20.588	34.192 50.55	
ANISOU 305	CG ASP	36 2537	1818 4402	-175 -833 - 208

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- 26 -ANISOU 397  $\circ$ ASP 49 3177 2863 4257 -368 1004 - 1544 MOTA 398 ASP CВ 49 -2.03434.824 60.167 1.000 30.34 ANISOU 398 CB ASP 3695 49 3210 4623 -559 713 -2178 ATOM 399 CG ASP -0.924 49 61.128 1.000 37.18 35.181 ANISOU 399 ASP CG 49 5259 4057 -1109 -211 -2007 4810 ATOM OD1 ASP 400 49 -0.55661.904 1.000 33.36 34.266 ANISOU 400 OD1 ASP 49 3717 4549 4408 -737 888 -1727 ATOM 401 OD2 ASP 49 36.375 -0.52561.087 1.000 48.45 OD2 ASP ANISOU 401 49 7960 3575 6875 -927 -2887 - 2409ATOM 402 N LEU. 50 .-3.788 33.402 58.059 1.000 24.46 ANISOU 402 NLEU 50 3114 2668 3513 374 200 -1298 ATOM 403 CALEU 50 -5.123 57.471 1.000 22.92 33.344 ANISOU 403 LEU CA50 2949 2145 3614 161 397 - 562 ATOM 404  $\mathsf{C}$ LEU 31.937 50 -5.67957.328 1.000 21.79 ANISOU 404  $\mathsf{C}$ LEU 50 3345 2197 2737 33 417 - 556 ATOM 405 0 LEU 50 -6.878 57.475 1.000 24.96 31.741 ANISOU 405 0 LEU 50 3463 2502 3517 766 -1181 -276 ATOM 406 LEU CB 50 -5.25434.137 56.194 1.000 22.13 ANISOU 406 CB LEU 50 3127 2016 3266 524 -757 -103 ATOM 407 CGLEU 50 -6.661 34.578 55.807 1.000 28.87 ANISOU 407 CG LEU 50 3549 3881 3538 961 825 208 ATOM 408 CD1 LEU 50 -7.38935.082 57.049 1.000 52.72 ANISOU 408 CD1 LEU 4567 50 8556 6907 940 2929 - 1936 CD2 LEU ATOM 409 50 -6.64435.642 54.723 1.000 41.07 CD2 LEU ANISOU 409 3395 6971 50 -1005 -2258 857 5240 ATOM 410 VAL  $\mathbf{N}$ 51 -4.801 30.956 57.138 1.000 21.78 ANISOU 410 VAL N 51 3345 2052 2877 -160 216 - 860ATOM 411 51 3-5.293 CA VAL 57.118 1.000 19.40 29.580 ANISOU 411 VAL CA 51 2683 2631 2056 -12173 - 303 412 ATOM C VAL -5.63151 29.135 58.533 1.000 25.25 ANISOU 412 C VAL 51 4453 2656 2485 587 - 955 -753 413 ATOM 0 VAL -6.652 51 58.725 1.000 25.07 28.454 ANISOU 413 VAL 51 0 4555 2176 2795 -484 1185 - 827 ATOM 414 CB VAL 28.589 -4.37751 56.396 1.000 18.78 ANISOU 414 CB VAL 51 2729 1786 2620 171 - 313-72ATOM 415 CG1 VAL 51 -3.15228.238 57.231 1.000 20.42 ANISOU 415 CG1 VAL 3002 51 1841 2918 295 -13 - 480CG2 VAL ATOM 416 51 -5:147 56.021 1.000 24.10 27.306 ANISOU 416 CG2 VAL 51 3112 2337 355 -846 3708 -511 ATOM 417 ILE N 52 -4.83629.500 59.534 1.000 25.23 ANISOU 417 N ILE 52 4514 2471 2603 388 ATOM 418 -5.205 29.114 60.921 1.000 24.38 CA ILE 52 ANISOU 418 ILE CA52 3488 3010 2765 248 19 - 509 ATOM 419 ILE C 52 -6.498 61.355 1.000 24.20 29.771 ANISOU 419 ILE 52 3026 2482 3687 -354 114 -648ATOM 420 ILE 52 0 -7.328 62.071 1.000 27.73 29.182 ANISOU 420 ILE 0 52 3735 2812 -198 614 -334 3989 ATOM -4.016 421 CB ILE 52 29.427 61.829 1.000 27.59 ANISOU 421 ILE CB 3321 4347 52 2815 590 0 - 785 ATOM 422 CG1 ILE 52 -2.853 28.439 61.510 1.000 31.45 ANISOU 422 CG1 ILE 52 3278 5248 3425 741 363 -1288 ATOM 423 CG2 ILE 52 -4.29329.312 63.317 1.000 33.62 ANISOU 423 CG2 ILE 52 3827 6199 150 -1454 2750 881 CD1 ILE ATOM 424 52 -1.930 28.351 62.710 1.000 36.22 ANISOU 424 CD1 ILE 52 3956 5082 4722 979 -601 - 234ATOM 425 ASP N 53 -6.77130.992 60.913 1.000 24.56 ANISOU 425 3479 ASP N 53 2878 2974 165 609 - 426ATOM 426 53 CAASP -8.051 61.278 1.000 23.50 31.646 ANISOU 426 ASP CA53 3242 2942 2745 -5 355 -677 MOTA 427 C ASP 53 -9.201 30.929 60.594 1.000 26.34 ANISOU 427 ASP 53 3462 2986 -435 612 -1064 3561

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ATOM ANISOU	544		THR	67	-14.060	20.554	52.961		224 <b>-</b> 492 20 14
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ANISOU ATOM	546 547	N C 2	SER	68	1612	1720	3018	-135	154 - 498
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                      72
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ATOM
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ANISOU 576
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            OG1 THR
ATOM
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ANISOU 579
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MOTA
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            N
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                          -6.877
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						<b>-</b> 32 -			
ANISOU ATOM ANISOU	11223334455566778889900112233344555666666666666666666666666666666	NH2 NH2 NH NA NA CCCCCCCCCC NA NA NA NA NA NA NA NA NA NA NA NA NA	TTTTTTTTTTTTTTGGGGGGGGGGGGGGGGGGGGGGGG	777777777777777777777777777777777777777	2 - 1 - 1 - 1 - 2 - 3 - 4 - 2 - 1 - 1 - 1 - 2 - 3 - 4 - 2 - 1 - 1 - 1 - 2 - 3 - 4 - 2 - 1 - 1 - 2 - 3 - 4 - 2 - 1 - 3 - 3 - 2 - 3 - 4 - 3 - 3 - 3 - 4 - 3 - 3 - 3 - 3	1708 16.618 17.03 16.67 17.03 15.03 15.13 16.03 17.03 18.03 18.03 19.03 10	2638 39.987 2532 47.101 2507 46.980 2272 48.122 2414 48.460 3101 45.668 2317 44.441 2334 44.334 2475 43.011	88 -302 - 340 1.000 16.65 241 -162 - 420 1.000 19.39 -112 -240 - 540 1.000 20.56 345 -507 - 286 1.000 30.33 -69 -609 10 27 1.000 36.13 336 -918 15 96 1.000 58.07 975 -1592 - 31 1.000 16.83 -6 -211 131 1.000 15.87 -17 52 - 325 1.000 14.22 141 -32 - 42 1.000 15.45 -12 -46 - 73 1.000 15.68 160 -14 - 311 1.000 16.37 -181 -8 - 177 1.000 16.37 -181 -8 - 177 1.000 19.21 -142 241 - 156 1.000 17.00 -67 26 - 147 1.000 18.00 51 -66 - 220 1.000 20.50 -110 310 - 387 1.000 15.28 137 340 - 173 1.000 15.59 1.000 15.59 1.130 - 106 1.000 15.59 1.130 - 10 1.000 15.25	3 8
ATOM ANISOU ATOM ANISOU ATOM	604 604 605 605 606	CG CCD CD NE CZ NH1 NH2	ARG ARG ARG ARG ARG	75 75 75 75 75	-6.848 1495 -5.712 1658 -5.061	20.634 2110 21.618 1792 21.601	2317 44.441 2334 44.334 2475 43.011 2596 42.732 2221 43.664 2623 41.518 2232 48.651	1 46 - 106 1.000 15.63 9 147 2 2 0 1.000 15.59 11 130 - 1 0 1.000 15.25 122 227 1 4 4 1.000 14.90 71 -86 2 4 2 1.000 16.18 -134 -387 3 3 7 1.000 15.83 -193 221 0	

- 33 -ATOM 611 CAGLY 76 22.532 -8.858 49.637 1.000 16.67 ANISOU 611 CAGLY 1650 76 2260 2425 199 -612 -70 612 ATOM C GLY 76 -8.602 22.002 51.036 1.000 16.32 ANISOU 612 C GLY 1584 76 2014 2602 -126 268 -347 ATOM 613 0 GLY 76 -7.46921.651 51.370 1.000 16.87 ANISOU 613 GLY 0 1638 76 1998 2773 -45 308 -218 ATOM 614 N PHE 77 -9.643 51.863 1.000 16.88 22.025 ANISOU 614 1597 PHE 77 N 2141 -7 283 -191 2675 ATOM 615 CAPHE 77 -9.584 21.646 53.274 1.000 17.61 ANISOU 615 CA PHE 77 2196 1838 2656 109 328 -114 616 ATOM C PHE 77 -9.77653.512 1.000 17.64 20.154 ANISOU 616  $\mathsf{C}$ PHE 77 1855 2600 2248 -68 243 -185 ATOM 617 0 PHE 77 -10.589 19.528 52.831 1.000 18.23 ANISOU 617 PHE 0 77 1844 2488 2594 357 - 240 -183ATOM 618 CB PHE 77 -10.698 22.383 53.998 1.000 17.70 ANISOU 618 CB PHE 77 1730 2480 2515 65 - 344 162 ATOM 619 PHE CG -10.877 22.081 77 55.473 1.000 19.61 ANISOU 619 CG PHE 77 2405 2530 195 2515 261 -516 CD1 PHE 620 ATOM 77 -9.966 22.594 56.395 1.000 22.27 ANISOU 620 CD1 PHE 77 2514 3523 2426 431 -23 -527 MOTA 621 CD2 PHE 77 -11.917 21.285 55.94,1 1.000 21.31 ANISOU 621 CD2 PHE 3282 77 2070 2743 36 615 - 288 CE1 PHE 622 ATOM -10.116 22.294 77 57.742 1.000 21.05 ANISOU 622 CE1 PHE 77 2719 2768 2510 171 221 - 339623 ATOM CE2 PHE 77 -12.079 20.991 57.300 1.000 25.09 ANISOU 623 CE2 PHE 77 2967 4120 2447 -501 625 -826 624 ATOM PHE CZ-11.175 21.523 77 58.207 1.000 23.79 ANISOU 624 CZPHE 77 2263 3681 3095 -1 376 -756ATOM 625 9.022 Ν THR 78 54.490 1.000 17.64 19.631 ANISOU 625 THR 1616  $\mathbf{N}$ 78 2161 2925 37 336 1 ATOM 626 THR CA78 54.983 1.000 18.12 -9.29618.279 ANISOU 626 CA THR 78 1926 2243 -157 2717 624 - 28 ATOM 627 C THR 78 -9.291 56.505 1.000 18.66 18.316 ANISOU 627 C THR 78 2120 2663 2308 -367 519 - 288 628 ATOM THR 0 78 -8.335 18.821 57.095 1.000 21.42 ANISOU 628 Q THR 78 3098 2158 2883. -43290 1 7 7 ATOM 629 THR CB78 -8.25217.242 54.521 1.000 21.00 ANISOU 629 CB THR 78 2973 2067 2939 113 428 - 574630 ATOM OG1 THR 78 17.392 -8.02753.104 1.000 21.18 ANISOU 630 OG1 THR 78 2544 2671 2833 160 317 - 773 ATOM CG2 THR 631 15.832 78 -8.735 54.800 1.000 26.65 CG2 THR ANISOU 631 3759 78 2227 4141 -275 853 -618 ATOM 632 -10.311 17.804 N GLY 79 57.181 1.000 20.36 ANISOU 632 GLY N 2669 79 2379 2690  $-670 \cdot 630 - 144$ ATOM 633 GLY -10.344 17.679 CA79 58.623 1.000 25.96 ANISOU 633 CA GLY 79 3871 3249 2745 -790 576 375 ATOM 634 C GLY -10.029 16.238 59.039 1.000 39.70 79 ANISOU 634 C GLY 79 6407 3542 5135 -1658 -1944 1511 ATOM 635 GLY -10.623 15.303 0 79 58.491 1.000 31.02 ANISOU 635 0 GLY 79 4327 3187 4272 -404 419 - 75ATOM 636 LEU N 80 -9.069 59.936 1.000 36.07 16.055 ANISOU 636 N LEU 80 4380 4536 4788 1381 -564 - 835ATOM 637 LEU CA -8.63480 14.713 60.340 1.000 32.52 ANISOU 637 CALEU 3640 80 4083 4632 611 -502 -898 ATOM 638 C LEU 80 -9.131 14.311 61.716 1.000 39.82 ANISOU 638 C LEU 5051 80 4652 5428 -128 418 -538 ATOM 639 0 LEU 80 -9.998 62.305 1.000 37.05 14.963 ANISOU 639 LEU 5057 80 3807 5213 -292 666 8 7 ATOM 640 CB LEU 80 -7.12260.265 1.000 38.36 14.580 ANISOU 640 CB LEU 3821 80 5456 5299 1568 -33 -1406 ATOM - 641 CG LEU -6.488 80 14.753 58.883 1.000 38.27

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                                   8505
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                                                    -1092 - 76
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        643
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ATOM
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                          3172
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                                            2787
                                                    -275
                                                          739 - 782
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ATOM
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ATOM
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ANISOU 670
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             CE1 TYR
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             CE2 TYR
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                                            3108
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ATOM
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MOTA
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            OG1 THR
       699
                      105 -0.865
                                   23.675
                                            38.217 1.000 18.66
ANISOU 699
            OG1 THR
                                   2449
                      105 2035
                                            2607
                                                   -140
                                                         -458 4 1 6
ATOM
            CG2 THR
       700
                      105 1.155
                                   24.590
                                            39.178 1.000 18.95
ANISOU 700
            CG2 THR
                      105 1748
                                   2853
                                            2601
                                                   -105 -248 2 9 6
MOTA
       701
                ALA
            N
                      106 -3.507
                                   24.751
                                            39.741 1.000 16.52
ANISOU 701
                ALA
                      106 1596
            N
                                   2293
                                                   -180 -1 2 9 8
                                            2389
ATOM
       702
                ALA
                      106 -4.846
            CA
                                   25.035
                                            39.218 1.000 16.59
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- 36 -
ANISOU 702
             CA
                 ALA
                      106 1692
                                   1952
                                            2660
                                                   -214
                                                         -209243
        703
ATOM
             C
                 ALA
                      106 -5.848
                                   24.142
                                           39.923 1.000 17.52
ANISOU 703
             C
                 ALA
                       106 1651
                                   1821
                                                   26 -66 5 5 5
                                            3186
        704
ATOM
             0
                 ALA
                      106 - 5.479
                                           40.805 1.000 17.88
                                   23.323
ANISOU 704
             0
                 ALA
                      106 2038
                                   2087
                                           2668
                                                   59 -51 3 8 8
ATOM
        705
             CB
                 ALA
                      106 -4.862
                                   24.838
                                           37.713 1.000 20.31
ANISOU 705
             CB
                 ALA
                      106 2331
                                   2764
                                           2620
                                                   -197
                                                         -403440
MOTA
        706
                 ASP
                      107 -7.149
             N
                                           39.717 1.000 18.00
                                   24.329
ANISOU 706
                 ASP
             N
                      107 1576
                                   2208
                                           3057
                                                   -77
                                                         -12049
ATOM
        707
             CA
                      107 -8.217
                 ASP
                                   23.535
                                           40.344 1.000 17.46
ANISOU 707
             CA
                 ASP
                      107 1563
                                   2191
                                           2881
                                                   -83
                                                         -472 3 6 3
ATOM
        708
             C
                 ASP
                                  .23.753
                      107 - 8.173
                                           41.859 1.000 17.74
             \mathsf{C}
ANISOU 708
                      107 1825
                 ASP
                                   2044
                                           2869
                                                   447
                                                         -269 3 6 2
ATOM
        709
             0
                 ASP
                      107 -8.458
                                   22.854
                                           42.650 1.000 18.95
ANISOU 709
                      107 1994
                 ASP
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                                                   167
                                                         -133 4 0 2
ATOM
        710
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             CB
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                                           39.990 1.000 19.62
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ANISOU 710
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                 ASP
                      107 2213
                                   2300
                                           2942
                                                   -394
                                                         -727173
       711
ATOM
             CG
                 ASP
                      107 - 8.370
                                   21.842
                                           38.508 1.000 20.81
ANISOU 711
                      107 1952
             CG
                 ASP
                                   3093
                                                   -138
                                           2862
                                                         -532 - 14
ATOM
       712
             OD1 ASP
                      107 - 9.369
                                   22.369
                                           37.976 1.000 25.84
             OD1 ASP
ANISOU 712
                      107 2524
                                   3967
                                           3327
                                                   222
                                                         -1149 - 240
             OD2 ASP
       713
ATOM
                      107 - 7.544
                                   21.168
                                           37.844 1.000 25.86
ANISOU 713
             OD2 ASP
                      107 3314
                                           3523
                                   2989
                                                   391
                                                         -91
                                                             - 8 9
ATOM
       714
                 ASN
             Ν
                                   24.962
                      108 - 7.893
                                           42.298 1.000 18.18
ANISOU 714
                 ASN
             N
                      108 2049
                                   2075
                                                         189
                                           2786
                                                   509
                                                             153
ATOM
       715
             CA
                      108 -7.831
                 ASN
                                   25.263
                                           43.740 1.000 17.10
ANISOU 715
             CA
                ASN
                      108 1804
                                           2715
                                   1977
                                                   266
                                                         291
                                                             3 2 7
ATOM
       716
             C
                 ASN
                      108 -9.158
                                   25.716
                                           44.314 1.000 17.11
ANISOU 716
             C
                 ASN
                      108 1705
                                   2061
                                           2734
                                                         44 1 4 9
                                                   367
ATOM
       717
                      108 -10.103 26.086
             0
                 ASN
                                           43.604 1.000 20.72
ANISOU 717
             0
                 ASN
                      108 2066
                                   2377
                                           3430
                                                   759
                                                         -248245
ATOM
       718
             CB
                 ASN
                      108 - 6.799
                                  26.379
                                           43.969 1.000 19.90
ANISOU 718
             CB
                 ASN
                      108 1770
                                   2308
                                           3483
                                                   186
                                                         298 - 171
ATOM
       719
             CG
                 ASN
                                   25.862
                      108 -5.400
                                           43.717 1.000 17.24
ANISOU 719
             CG
                 ASN
                      108 1709
                                   2212
                                           2628
                                                         68 1 8 4
                                                   200
ATOM
       720
            OD1 ASN
                                   24.850
                      108 - 4.986
                                           44.277 1.000 17.42
ANISOU 720
                      108 2003
            OD1 ASN
                                   1984
                                           2631
                                                   109
                                                         11 - 62
ATOM
       721
            ND2 ASN
                      108 -4:644
                                  26.487
                                           42.834 1.000 18.41
ANISOU 721
                      108 2083
            ND2 ASN
                                   2326
                                           2587
                                                   -82
                                                         300 - 18
       722
ATOM
                      109 -9.308
                 LEU
            N
                                  25.509
                                           45.607 1.000 18.09
ANISOU 722 N LEU 109 1795 2294
                                           2786
                                                  349
                                                         344 1 0
ATOM
       723
            CA LEU
                      109 -10.532 25.803
                                           46.369 1.000 19.11
ANISOU 723
                      109 1763
            CA
                LEU
                                  2200
                                           3296
                                                  14 476 - 598
ATOM
       724
                      109 -10.169 26.790
            C
                LEU
                                           47.457 1.000 17.40
ANISOU 724
            C
                LEU
                      109 1682
                                   1937
                                           2990
                                                   251
                                                         129 - 207
MOTA
       725
                      109 -9.443 26.423
                LEU
             0
                                           48.395 1.000 21.18
ANISOU 725
                LEU
                      109 2443
             0
                                  1922
                                           3684
                                                  174
                                                         -520 2
ATOM
       726
                      109 -11.100 24.504
                LEU
            CB
                                           46.940 1.000 17.10
ANISOU 726
            CB
                LEU
                      109 1888
                                  2142
                                           2469
                                                  199
                                                         426 - 630
ATOM
       727
            CG
               LEU
                      109 -11.520 23.425
                                           45.944 1.000 18.07
ANISOU 727
            CG LEU
                      109 2515
                                   1943
                                           2409
                                                  190
                                                         -198 - 363
            CD1 LEU
ATOM
       728
                      109 -11.895 22.124
                                          46.654 1.000 20.06
ANISOU 728
            CD1 LEU
                      109 2842
                                   2406
                                                  -331 -175 -200
                                           2375
ATOM
       729
            CD2 LEU
                      109 -12.630 23.908
                                           45.035 1.000 25.24
ANISOU 729
            CD2 LEU
                      109 3481
                                   2892
                                           3217
                                                   306
                                                         -992 - 111
ATOM
       730
                 PHE
                      110 -10.609 28.036
            N
                                           47.313 1.000 17.25
ANISOU 730
                 PHE
            И
                      110 1584
                                   1926
                                           3045
                                                   272
                                                         184 - 132
ATOM
       731
                      110 -10.235 29.071
                PHE
             CA
                                           48.277 1.000 18.20
ANISOU 731
            CA PHE
                      110 1751
                                           3346
                                   1816
                                                   169
                                                         221 - 160
ATOM
       732
                 PHE
                      110 -11.409 29.567
             C
                                           49.106 1.000 19.93
ANISOU 732
             C
                 PHE
                      110 2077
                                   1609
                                           3886
                                                   71 650 - 335
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MOTA

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CA PHE

- 37 -110 -12.433 29.948 ATOM 733 PHE 0 48.494 1.000 24.64 ANISOU 733 110 2051 0 PHE 2461 4851 612 328 - 779 MOTA 734 CB PHE 110 - 9.60730.243 47.520 1.000 19.92 ANISOU 734 PHE CB 110 2367 1876 3324 224 - 9 3 619 ATOM 735 CG PHE 110 - 8.38029.986 46.688 1.000 19.47 ANISOU 735 PHE 110 2009 CG 2209 3179 327 - 791 -321 ATOM 736 CD1 PHE 110 -7.177 29.680 47.287 1.000 20.59 ANISOU 736 CD1 PHE 110 2071 2080 3674 -274 236 - 331 110 -8.437 ATOM 737 CD2 PHE 30.035 45.299 1.000 20.19 ANISOU 737 CD2 PHE 110 2557 1914 3200 543 - 289 112 ATOM 738 CE1 PHE 110 -6.034 29.454 46.559 1.000 21.06 CE1 PHE ANISOU 738 2309 110 2020 3673 -386 165 -622 ATOM 739 CE2 PHE 110 -7.277 29.811 44.547 1.000 20.77 CE2 PHE ANISOU 739 110 2495 2138 3257 197 504 - 398 ATOM 740 CZ110 -6.081 PHE 29.518 45.175 1.000 22.42 ANISOU 740 110 2747 PHE CZ2092 3678 531 339 - 357 ATOM 741 111 -11.238 29.718  $\mathbf{N}$ PRO 50.416 1.000 22.11 ANISOU 741 Ν PRO 111 2250 2153 3996 -72 871 -620 ATOM 742 111 -12.287 30.389 CAPRO 51.195 1.000 28.23 ANISOU 742 PRO CA111 3895 2210 4621 698 1514 - 671 ATOM 743 C PRO 111 -12.333 31.866 50.784 1.000 30.57 ANISOU 743 C PRO 111 4528 2026 5061 410 -1041 410 ATOM 744 111 -11.390 32.340 0 PRO 50.115 1.000 31.71 ANISOU 744 0 PRO 111 4040 2236 5774 -179 -597 - 1 2 ATOM 745 PRO CB 111 -11.799 30.250 52.627 1.000 33.20 ANISOU 745 CB PRO 2702 111 5609 4303 671 1671 - 790 ATOM 746 CG 111 -10.646 29.326 PRO 52.647 1.000 26.04 ANISOU 746 CG PRO 111 2742 3316 3835 1324 - 192 -931 ATOM 747 CD PRO 111<sup>2</sup>-10.161 29.149 51.230 1.000 22.15 ANISOU 747 CD PRO 111 2587 2307 3522 541 - 623 -471 ATOM 748 Ν SER 112 -13.337 32.641 51.150 1.000 42.13 ANISOU 748 N 112 7176 SER 2716 6115 2074 1731 - 526 ATOM 749 CA SER 112 -13.368 34.026 50.672 1.000 44.05 ANISOU 749 112 6799 CA SER 2255 7684 1107 -485 -826 ATOM 750 C SER 112 -13.262 34.157 49.149 1.000 68.28 ANISOU 750 C SER 112 13632 4498. 7812 -1855 -2077 1301 751 MOTA 112 -12.347 34.825 0 SER 48.646 1.000 95.18 ANISOU 751 112 15991 0 SER 11425 8747 -4337 -70 1985 ATOM 752 SER 112 -12.493 35.069 CB 51.349 1.000 39.31 ANISOU 752 112 2247 CB SER 4535 8153 580 1662 - 1437 ATOM 753 112 -11.474 34.624 OG SER 52.213 1.000 37.49 ANISOU 753 OG SER 112 7213 806 2453 4579 747 -1152 ATOM 754 ASP 114 -9.515 37.322 49.945 1.000 36.40 N ANISOU 754 N ASP 114 3476 2118 1254 403 1484 8237 MOTA 755 CA ASP 114 -8.205 37.586 50.600 1.000 30.79 ANISOU 755 CA ASP 114 3503 2856 5340 1229 1240 9 9 6 ATOM 756 114 -7.242 C ASP 36.402 50.648 1.000 26.16 ANISOU 756 C 114 2581 ASP 2404 4955 601 1114 8 0 4 ATOM 757 ASP 114 -6.031 36.458 50.338 1.000 25.45 ANISOU 757 ASP 114 2302 2503 4866 -43 602 131 ATOM 758 CB ASP 114 -8.595 52.075 1.000 43.68 37.874 ANISOU 758 114 7509 ASP CB 2783 1157 2727 - 210 6304 759 ATOM CG ASP 114 -7.391 38.386 52.835 1.000 46.96 ANISOU 759 CG ASP 114 9259 3225 5359 2517 519 107 ATOM 760 OD1 ASP 114 -6.487 52.189 1.000 83.49 38.959 ANISOU 760 OD1 ASP 114 13724 9866 8132 -6354 650 -3056 ATOM 761 OD2 ASP 114 -7.370 38.262 54.071 1.000113.59 ANISOU 761 OD2 ASP 114 27880 10550 4730 -6984 - 159 - 2575ATOM 762 PHE 115 -7.831 35.323  $\mathbf{N}$ 51.153 1.000 22.32 ANISOU 762 N PHE 115 2620 2062 3799 954 - 114 204

115 -7.115 34.026

51.183 1.000 22.69

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- 38 -ANISOU 763 115 2765 PHE 1909 CA 3947 118 1093 - 187 ATOM 764 115 -6.502 C PHE 33.754 49.816 1.000 21.49 ANISOU 764 115 2146 C PHE 2316 3702 559 - 255 305 ATOM 765 PHE 0 115 -5.328 33.362 49.758 1.000 20.51 ANISOU 765 0 PHE 115 2153 2011 3627 323 488 - 158 ATOM 766 PHE CB115 -8.096 32.928 51.638 1.000 20.76 ANISOU 766 115 2369 PHE CB 3574 1946 -3 563 - 473 ATOM 767 CG PHE 115 - 7.49631.590 51.998 1.000 20.23 ANISOU 767 CG PHE 115 2369 1854 3463 -155 629 - 377768 CD1 PHE ATOM 115 -6.915 30.756 51.041 1.000 20.35 CD1 PHE ANISOU 768 115 2572 1786 3372 -195 112 - 756 CD2 PHE 769 ATOM 115 -7.474 31.152 53.309 1.000 21.11 ANISOU 769 CD2 PHE 115 2802 1932 3287 -113 17 - 689 770 CE1 PHE ATOM 115 -6.351 29.538 51.325 1.000 21.09 CE1 PHE ANISOU 770 115 2502 1728 3784 -295 471 - 538 CE2 PHE ATOM 115 -6.938 771 29.901 53.623 1.000 27.40 CE2 PHE ANISOU 771 115 5012 1955 3445 444 43 - 572MOTA 772 CZPHE 115 -6.332 52.655 1.000 24.92 29.110 ANISOU 772 115 3356 CZPHE 1889 4222 50 1519 2 2 1 773 ATOM N GLU 116 -7.301 33.768 48.757 1.000 21.64 ANISOU 773 GLU N 116 2396 1835 3990 338 261 - 13ATOM 774 CA116 -6.750 GLU 33.424 47.444 1.000 20.90 ANISOU 774 CAGLU 116 2235 1965 3742 224 74 1 1 6 775 ATOM C GLU 116 -5.550 34.262 47.054 1.000 20.32 ANISOU 775  $\mathsf{C}$ GLU 116 1978 1899 3845 439 -108 4 4 8 ATOM 776 GLU 0 116 - 4.54433.679 46.604 1.000 20.18 ANISOU 776 GLU 0 116 2209 3312 2147 424 73 1 3 9 ATOM CB 777 GLU 116 -7.851 46.385 1.000 24.22 33.561 ANISOU 777 CB 116 2425 GLU 2638 4139 -467 -237 5 1 9 778 ATOM CG GLU 116 -7.339 33.331 44.980 1.000 23.27 ANISOU 778 116 2425 CG GLU 2465 3952 -7 - 494750 ATOM 779 CDGLU 116 -8.401 33.273 43.910 1.000 25.02 ANISOU 779 CD GLU 116 2695 2703 -510 -739 1509 4107 780 OE1 GLU ATOM 116 -9.617 33.306 44.207 1.000 34.83 ANISOU 7.80 OE1 GLU 116 2466 4606 -203 -928 1566 6161 781 OE2 GLU ATOM 116 -8.001 33.030 42.763 1.000 40.92 OE2 GLU ANISOU 781 116 4389 7172 3988 -24 -968 6 9 3 ATOM 782 ARG N 117 -5.549 35.571 47.300 1.000 20.60 ANISOU 782 NARG 117 2299 1811 3718 382 -10 469 ATOM 783 CAARG 117 - 4.37446.866 1.000 22.65 36.374 ANISOU 783 CA ARG 117 2230 1791 4586 351 107 153 784 C ATOM ARG 117 -3.163 35.911 47.648 1.000 21.87 ANISOU 784 C ARG 117 2269 1865 4178 252 179 9 7 785 ATOM 117 -2.060 35.789 ARG 0 47.102 1.000 22.10 ANISOU 785 ARG 0 117 2197 3931 2270 216 41 2 0 5 786 - CB ATOM ARG 117 -4.682 37.861 47.105 1.000 29.47 ANISOU 786 CB ARG 117 2849 1691 6658 259 -555 - 1ATOM 787 117 -3.485 CG ARG 38.815 47.046 1.000 40.24 ANISOU 787 ARG 117 3905 CG 2567 -819 -1330 -476 8818 ATOM 788 CD ARG 117 - 3.74540.160 47.716 1.000 52.75 ANISOU 788 CD ARG 2848 117 4698 12496 -595 -1653 -1669 789 ATOM ARG ΝE 117 - 3.93439.987 49.155 1.000 68.00 ANISOU 789 ARG ΝE 4719 117 8247 12872 422 1842 - 3441 ATOM 790 CZARG 117 -3.166 40.448 50.126 1.000 78.38 ANISOU 790 CZ117 13026 ARG 5658 11097 283 448 - 2498 NH1 ARG ATOM 791 117 -2.097 41.186 49.849 1.000 89.01 ANISOU 791 NH1 ARG 117 14218 11488 8115 -3550 -6761 3577 NH2 ARG ATOM 792 117 -3.479 40.189 51.391 1.000 82.58 ANISOU 792 NH2 ARG 117 16575 2856 11947 2617 2551 - 2095 ATOM 793 118 -3.334 35.759 N ILE 48.954 1.000 21.70 ANISOU 793 ILE N 118 2319 1797 4127 311 271 - 314

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- 39 -ATOM 794 118 -2.206 CAILE 35.425 49.810 1.000 20.99 ANISOU 794 CAILE 118 2546 1624 3805 408 294 - 470 118 -1.596 ATOM 795 C ILE 49.475 1.000 18.79 34.073 ANISOU 795 C ILE 118 2222 1534 573 - 201 3384 218 796 ATOM ILE 33.858 0 118 - 0.40949.323 1.000 17.27 ANISOU 796 0 ILE 118 2194 1663 2707 351 - 136 283 797 ATOM ILE CB 118 -2.588 35.542 51.293 1.000 22.62 ANISOU 797 ILE CB 118 2702 1997 3895 276 416 -856 118 -2.916 MOTA 798 CG1 ILE 51.700 1.000 27.54 36.995 CG1 ILE ANISOU 798 118 5077 1801 3587 503 768 799 ATOM CG2 ILE 118 -1.552 34.940 52.206 1.000 23.59 CG2 ILE ANISOU 799 118 3084 2274 3606 183 254 - 818 118 -3.493 MOTA 800 CD1 ILE 37.115 53.096 1.000 29.35 CD1 ILE ANISOU 800 118 5212 2054 3885 558 1114 - 645 MOTA 801 TRP N 119 - 2.45433.069 49.341 1.000 17.93 ANISOU 801 119 2378 TRP N 1605 2828 147 -80 -2.69 802 119 -2.035 ATOM TRP CA31.688 49.103 1.000 16.57 ANISOU 802 CATRP 119 2126 1538 2630 152 -25 - 1 6 ATOM 803 C TRP 119 -1.575 31.476 47.676 1.000 16.98 ANISOU 803 C TRP 119 2126 1723 2604 269 -91 - 51 ATOM 804 0 30.640 TRP 119 - 0.70047.455 1.000 17.58 ANISOU 804 1674 0 TRP 119 1892 3113 181 135 ATOM 805 119 -3.127 CB TRP 30.690 49.591 1.000 18.32 ANISOU 805 TRP 1789 CB119 2156 3014 -34 5 ATOM 806 CG TRP 119 -2.934 30.457 51.082 1.000 18.27 ANISOU 806 TRP CG 119 2208 1711 3025 86 349 5 6 MOTA 807 CD1 TRP 119 -3.354 52.103 1.000 20.36 31.273 ANISOU 807 CD1 TRP 119 2624 2029 3083 156 276 - 1 5 3 808 ATOM CD2 TRP  $119^3 - 2.213$ 29.383 51.683 1.000 18.61 ANISOU 808 CD2 TRP 119 2049 2055 2967 134 263 NE1 TRP ATOM 809 119 -2.955 53.323 1.000 20.55 30.773 ANISOU 809 119 2471 NE1 TRP 3109 2229 92 266 - 106 ATOM 810 CE2 TRP 119 -2.260 29.603 53.073 1.000 20.21 CE2 TRP ANISOU 810 119 2529 2258 2893 180 754 CE3 TRP ATOM 811 119 -1.576 28.258 51.147 1.000 18.29 ANISOU 811 CE3 TRP 119 2258 1714 2977 42 - 70 - 20812 ATOM CZ2 TRP 119 -1.636 53.981 1.000 21.97 28.728 ANISOU 812 CZ2 TRP 119 2876 2526 2945 384 51 - 106 CZ3 TRP ATOM 813 119 -0.968 52.045 1.000 19.35 27.375 CZ3 TRP ANISOU 813 119 2576 2028 2750 187 415 814 ATOM CH2 TRP 27.618 119 -1.026 53.442 1.000 21.67 CH2 TRP ANISOU 814 119 3033 250 9 7 2379 2823 350 ATOM 815 120 -2.129 THR 32.192 N 46.701 1.000 16.93 ANISOU 815 N THR 120 2023 1833 2577 122 -112 1 8 ATOM 816 CA THR 120 -1.598 45.342 1.000 17.85 32.086 ANISOU 816 120 1915 CATHR 2469 -371 - 3242398 222 ATOM 817 THR 120 -0.169 C 45.288 1.000 17.15 32.587 ANISOU 817 C THR 120 2031 1855 2629 241 -155 1 9 2 ATOM 818 0 THR 120 0.700 44.674 1.000 18.67 31.960 ANISOU 818 120 1996 THR 0 1887 389 3212 -131 1 7 7 ATOM 819 120 -2.487 THR CB 44.344 1.000 18.10 32.865 ANISOU 819 THR CB 120 1951 2204 2720 28 -93 3 4 5 ATOM 820 OG1 THR 120 -3.773 32.238 44.284 1.000 20.49 ANISOU 820 OG1 THR 120 1807 3179 59 - 363 558 2801 ATOM 821 CG2 THR 120 -1.919 32.803 42.933 1.000 22.46 ANISOU 821 CG2 THR 120 2438 3266 2830 475 118 705 ATOM 822 GLN N 121 0.094 33.708 45.956 1.000 18.62 ANISOU 822 GLN N 121 2180 1657 3237 123 -94 213 ATOM 823 121 1.466 GLN CA34.232 45.993 1.000 18.15 ANISOU 823 CA GLN 121 2077 1698 3119 77 96 5 2 0 824 ATOM C GLN 33.284 121 2.412 46.718 1.000 17.04

						- 40 -			
ANISOU	_	С	GLN		2022	1431	3019	192	234 223
ATOM	825	0	GLN		3.510	33.047	46.270		19.32
ANISOU		0	GLN		1894	1800	3645	93 24	6 1 2 9
ATOM ANISOU	826	CB	GLN	121		35.579	46.756	1.000	22.90
ATOM	826 827	CB	GLN		2520	1479	4702	327	-812 2 7 1
ANISOU		CG CG	GLN GLN		2.888	36.159	46.871		27.04
ATOM	828	CD	GLN		2949	2062	5262	-346	-400 1 3 2
ANISOU	828	CD	GLN		3.530 3307	36.511	45.535		
ATOM	829		GLN		466.0	2733 36.085	6097 45.247	983	1031 9 9
ANISOU	829	=	GLN		3009	9570	11267	1.000 1758	
MOTA	830	NE2	GLN		2.859	37.306	44.716	1.000	2366 2029 55.89
ANISOU	830	NE2	GLN	121	6516	7728	6993	2815	1745 3249
ATOM	831	N	TYR		1.997	32.791	47.871		16.87
ANISOU	831	N	TYR		2389	1518	2501	71 -1	
ATOM ANISOU	832 832	CA	TYR		2.795	31.881	48.683	1.000	17.97
ATOM	833	CA C	TYR TYR		2564	1600	2666	176	-224 - 56
ANISOU	833	C	TYR		3.080 1870	30.600	47.909	· · · - •	16.83
ATOM	834	Õ	TYR		4.224	1460 30.129	3065	-31	-57 - 98
ANISOU	834	0	TYR		1891	1952	47.823 2872	1.000	17.67 -220 1 2 6
ATOM	835	CB	TYR	122		31.522	49.960		18.01
ANISOU	835	CB	TYR		2526	1821	2495	2 -3	
ATOM	836	CG	TYR		2.753	30.619		-	17.89
ANISOU ATOM	836 837	CG CD1	TYR TYR		2332	1695	2769		-147 - 51
ANISOU	837		TYR		4.058 2883	30.901			21.71
ATOM	838		TYR		2.107	2101 29.496	3267	-257	-913 3 4
ANISOU	838		TYR		2428	2026	3634	128	21.29 -267 4 6 8
ATOM	839		TYR		4.680	30.037			21.27
ANISOU	839		TYR		2681	2045	3356	140	-725 - 210
ATOM ANISOU	840		TYR		2.746	28.637	52.290		24.50
ATOM	840 841	CE2 CZ	TYR TYR		3376	1876	4057		-1163 506
ANISOU	841	CZ	TYR		4.043 3161		=		22.16
ATOM	842	OH	TYR		4.699	1881 28.079	3379	95 -9	
ANISOU	842	ОН	TYR		3471	2398	3142		23.72 005 - 56
ATOM	843	N	PHE		2.074				16.21
ANISOU	843	N	PHE		1794	1571	2793		6 - 5 4
ATOM	844	CA	PHE		2.347	28.843	46.397		15.71
ANISOU ATOM	844 845	CA	PHE		1622	1800	2548		42 - 103
ANISOU	845	C	PHE PHE		3.378 1681	29.188	45.337		15.96
ATOM	846	Õ	PHE		4.276	1304 28.375	3078	42 90	
ANISOU	846	Ō	PHE		1703	1437	45.037 2739	54 14	15.47
ATOM	847	CB	PHE		1.036	28.309			15.07
ANISOU	847	CB	PHE	123	1460	1364	2904	209	-148 1
ATOM	848	CG	PHE		1.241	27.104			17.41
ANISOU ATOM	848 849	CG CD1	PHE		2090	1620	2906		-179 - 238
ANISOU	849		PHE PHE		1.170 1680	25.831			17.41
ATOM	850		PHE		1.490	1439 27.259	43.513		19 - 255
ANISOU	850		PHE		1723	2331	2870		18.22 -216 - 372
ATOM	851		PHE	123	1.419	24.740			19.15
	851		PHE		2112	1766	3397		
ATOM ANISOU	852 852		PHE		1.722	26.144	42.717	1.000	19.63
ATOM	853	CE2 CZ	PHE PHE		1901 1.635	2476	3083		-261 -632
ANISOU	853	CZ	PHE		1.635	24.868			19.40
ATOM	854	N	ASP		3.164	2424 30.304	3421 44.636	385	-529 - 490 16.86
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WO 99/33994			PCT/GB98/03860
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ATOM 949	CG ARG 135 17.571	1640 2767	-4 -1480 6 1 4
ANISOU 949	CG ARG 135 5112		
ATOM 950	CD ARG 135 16.930	2000	816 -610 5 9 5
ANISOU 950	CD ARG 135 3548	26.332 36.393 2428 2865	
ATOM 951	NE ARG 135 15.551		148 61 1371 1.000 22.68
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ATOM 952	CZ ARG 135 14.520		
ANISOU 952	CZ ARG 135 3801	2165 3874	921 -506 - 179
ATOM 953	NH1 ARG 135 14.708	27.515 37.702	1.000 23.50
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ATOM 954 ANISOU 954	NH2 ARG 135 13.287	<b>30.03</b> 3	1.000 24.30
ATOM 955	NH2 ARG 135 3520 N GLU 136 19 403	2441 3272	-101 72 5 8 2
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ATOM 957	C GLU 136 21.186	1770 2302	-97 279 140
ANISOU 957	C GLU 136 1535	150,570	1.000 16.74
ATOM 958	O GLU 136 22.350	~ — <b>-</b>	-148 - 172 - 72
ANISOU 958	O GLU 136 1710	1908 2999	1.000 17.42 7 30 9 2
ATOM 959	CB GLU 136 20.957		1.000 16.64
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ATOM 960	CG GLU 136:20.762	25.772 41.718	1.000 17.80
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ATOM	1087 1088	CD1	LEU		1893	2013	2135	-33 -186 - 36
ANISOU	1088	CDI	T.EU		13.922	22.829	36.614	1.000 18.41
ATOM	1089	CD2	LEU		1732 12.863	2473	2791	-156 80 -876
ANISOU	1089	CD2	LEU	153	3083	20.883 3182	37.794 2005	
ATOM	1090		ASP	154	8.473	21.866	34.708	365 261 193
ANISOU ATOM	1090		ASP	154	1768	1181	2525	1.000 14.41 -25 -8 2 9 3
ANISOU	1091 1091		ASP		7.092	22.373		1.000 15.90
ATOM	1091	CA	ASP ASP		1665	1615	2760	-195 27 769
ANISOU	1092	C			6.216 1859	21.161	34.814	1.000 14.66
ATOM	1093		ASP		5.995	1304	2409	-92 143 515
ANISOU	1093	0	ASP		2561	20.368 1455	33.889	1.000 17.30
ATOM	1094	CB	ASP		6.923	22.909		
ANISOU			ASP		1905	2077	3081	1.000 18.59 124 269 1317
ATOM ANISOU	1095		ASP		5.461			1.000 19.87
ATOM	1095		ASP		2029	2531	2990	226 129 1436
ANISOU	1096	ODI	ASP		4.561 1949	23.253	33.639	1.000 19.68
MOTA	1097	OD2	ASP		5.207	2209	3318	92 221 4 9 6
ANISOU	1097	OD2	ASP		2512	23.189 3475	31.554	1.000 23.73
ATOM	1098	N	CYS		5.831	_	3029 36.070	246 -137 653
ANISOU	1098	N	CYS		1708		2342	1.000 14.25 -101 -62 546
								02 340

- 49 -ATOM 1099 CA CYS 155 5.418 19.569 36.468 1.000 13.45 ANISOU 1099 CA CYS 155 1608 2158 1346 -191 4 4 5 8 1100 C ATOM CYS 155 4.157 37.302 1.000 12.49 19.574 ANISOU 1100 C CYS 155 1644 1331 1772 -200 -148 6 2 ATOM 1101 0 CYS 155 3.224 20.303 36.941 1.000 14.55 ANISOU 1101 O 155 1633 CYS 1492 2402 -111 4 4 2 -122 MOTA 1102 CB CYS 155 6.664 18.872 37.098 1.000 14.37 ANISOU 1102 CB CYS 155 1907 1366 2186 122 -137 2 1 1 1103 SG 155 7.265 ATOM CYS 19.595 38.641 1.000 14.99 ANISOU 1103 SG CYS 155 1561 1821 2315 -74 -98 182 1104 N ATOM GLU 18.706 156 4.060 38.316 1.000 12.89 ANISOU 1104 N GLU 156 1575 1379 1945 -130 29 1 9 4 1105 CA GLU ATOM 156 2.788 39.029 1.000 12.98 18.447 ANISOU 1105 CA GLU 156 1508 1311 2114 21 140 -2101106 C 156 2.987 ATOM GLU 18.676 40.510 1.000 12.34 GLU ANISOU 1106 C 156 1414 1198 24 204 2078 102 ATOM 1107 O 156 2.828 GLU 17.757 41.289 1.000 14.89 ANISOU 1107 O GLU 156 1875 1425 2359 -15 -54 442 ATOM GLU 1108 CB 156 2.278 38.678 1.000 14.48 17.047 ANISOU 1108 CB GLU 156 1968 1323 2213 -279 120 8 7 1109 CG ATOM GLU 156 1.855 17.038 37.227 1.000 14.86 ANISOU 1109 CG GLU 156 1894 1526 2227 -120 95 -152 ATOM 1110 CD 156 0.523 GLU 17.687 36.932 1.000 17.10 ANISOU 1110 CD GLU 156 2091 1976 44 -4 1 4 4 2431 ATOM 1111 OE1 GLU 156 -0.204 17.967 37.886 1.000 17.98 ANISOU 1111 OE1 GLU 156 1811 2155 2866 -35 10 - 355 1112 OE2 GLU ATOM 156 0.214 17.990 35.759 1.000 20.99 ANISOU 1112 OE2 GLU 2419 156*-*2854 2704 -386 -516 5 6 2 1113 N MOTA PRO 157 3.292 40.958 1.000 12.09 19.893 ANISOU 1113 N PRO 157 1314 1347 1934 12 -48 2 4 9 1114 CA ATOM PRO 157 3.576 42.391 1.000 13.28 20.121 ANISOU 1114 CA PRO 157 1425 1696 1924 -68 117 147 1115 C ATOM 157 2.330 PRO 43.248 1.000 12.87 19.996 ANISOU 1115 C 157 1236 PRO 1737 1916 -214 -47 124 157 1.192 ATOM 1116 0 PRO 42.744 1.000 13.73 20.190 ANISOU 1116 0 PRO 157 1286 1717 2214 -190 -17 143 ATOM 1117 CB 157 4.061 PRO 21.580 42.407 1.000 13.94 ANISOU 1117 CB 157 1518 PRO 1729 2047 -289 -166 2 4 7 ATOM 1118 CG PRO 157 3.363 22.184 41.226 1.000 13.06 ANISOU 1118 CG PRO 157 1558 1518 1887 -32 -158 - 88 1119 CD PRO 157 3.494 ATOM 21.128 40.167 1.000 12.03 ANISOU 1119 CD PRO 157 1521 1081 -2 -7 1 2 1 1968 1120 N ATOM LEU 158 2.542 19.738 44.526 1.000 13.02 ANISOU 1120 N LEU 158 1554 1493 1899 -124 148 7 3 MOTA 1121 CA LEU 158 1.438 19.699 45.496 1.000 12.72 ANISOU 1121 CA LEU 158 1465 1552 1815 -126 -14 3 6 ATOM 1122 C LEU 158 1.927 20.389 46.772 1.000 12.90 ANISOU 1122 C 158 1230 LEU 1715 1957 -27 -29 -80ATOM 1123 0 LEU 158 2.975 47.289 1.000 14.06 19.977 ANISOU 1123 O LEU 158 1374 2304 1666 59 -257 -236 ATOM 1124 CB LEU 158 1.046 18.244 45.815 1.000 13.58 ANISOU 1124 CB LEU 158 1673 1590 1896 -213 57 171 1125 CG ATOM 158 0.044 18.030 LEU 46.945 1.000 14.84 ANISOU 1125 CG LEU 158 1471 1774 2396 -16 262 242 1126 CD1 LEU ATOM 158 -1.333 46.671 1.000 16.96 18.635 ANISOU 1126 CD1 LEU 158 1485 2196 2764 5 -148 -401 1127 CD2 LEU ATOM 158 -0.142 47.161 1.000 14.98 16.539 ANISOU 1127 CD2 LEU 158 1976 1820 1897 -390 171 7 9 ATOM 1128 N 21.306 LEU 159 1.139 47.283 1.000 13.44 ANISOU 1128 N 159 1509 2165 LEU 1434 43 -87 -119 1129 CA LEU ATOM 159 1.443 48.571 1.000 13.39 21.963

- 50 -ANISOU 1129 CA LEU 159 1438 1555 2095 -36 -80 - 911130 C MOTA LEU 159 0.419 21.494 49.602 1.000 14.49 ANISOU 1130 C LEU 159 1336 2034 2135 -152 -20S - 38MOTA 1131 0 LEU 159 - 0.79021.596 49.419 1.000 15.09 ANISOU 1131 O 159 1414 LEU 1999 90 -131 2319 9 0 MOTA 1132 CB 159 1.390 LEU 23.466 48.394 1.000 15.28 ANISOU 1132 CB 159 1720 LEU 1447 2639 55 -325 -197 1133 CG ATOM 159 1.484 LEU 24.320 49.669 1.000 17.11 ANISOU 1133 CG 159 2146 LEU 2665 1689 363 -332 - 343 1134 CD1 LEU - 159 2.775 ATOM 24.114 50.453 1.000 18.70 ANISOU 1134 CD1 LEU 159 2276 1759 3070 379 -687 - 540 1135 CD2 LEU ATOM 159 1.312 25.801 49.291 1.000 21.00 ANISOU 1135 CD2 LEU 159 2918 1535 3526 439 -692 - 382 ATOM 1136 N ARG 160 0.916 21.107 50.774 1.000 14.37 ANISOU 1136 N 160 1688 ARG 1709 2063 -186 4 7 -101 1137 CA ATOM 160 0.055 ARG 20.747 51.901 1.000 15.61 ANISOU 1137 CA ARG 160 1726 1990 2217 -64 90 - 118 1138 C ATOM ARG 160 0.480 21.501 53.155 1.000 15.40 ANISOU 1138 C 160 1557 ARG 2158 2135 -34 -46 - 38ATOM 1139 0 160 1.639 ARG 21.401 53.576 1.000 16.32 ANISOU 1139 O 160 1528 ARG 2508 2164 63 41 - 104 ATOM 1140 CB ARG 160 0.048 19.263 52.227 1.000 16.13 ANISOU 1140 CB 160 2134 ARG 2084 1912 **-30**· 129 -127 1141 CG ATOM 160 -0.594 ARG 18.410 51.155 1.000 17.17 ANISOU 1141 CG ARG 160 1963 1934 2628 -140-212 - 60ATOM 1142 CD 160 -0.672 ARG 16.959 51.627 1.000 18.16 ANISOU 1142 CD ARG 160 2767 1965 2166 125 -330 - 351143 NE ATOM 160°-1.382 ARG 16.102 50.682 1.000 18.11 ANISOU 1143 NE ARG 160 2408 1775 2699 -56 -308201144 CZ ATOM 160 -1.221 ARG 14.789 50.581 1.000 16.76 ANISOU 1144 CZ ARG 160 2191 1748 2428 55 1 7 4 -97 1145 NH1 ARG ATOM 160 -0.326 51.374 1.000 20.55 14.192 ANISOU 1145 NH1 ARG 160 2306 2012 3491 -457 3 0 5 -26 1146 NH2 ARG ATOM 160 -1.908 14.095 49.689 1.000 19.23 ANISOU 1146 NH2 ARG 160 2502 2031 2774 -147 - 338 181 ATOM 1147 N 161 -0.469 PHE 22.257 53.755 1.000 15.36 ANISOU 1147 N PHE 161 1604 2120 2111 -37 -63 -128 ATOM 1148 CA PHE 161 -0.209 22.975 54.999 1.000 16.25 ANISOU 1148 CA 161 2173 PHE 1774 2227 -71 -187 - 891149 C ATOM PHE 161 -1.030 22.236 56.069 1.000 16.98 ANISOU 1149 C PHE 161 1980 2432 2041 -217 -161 - 162 ATOM 1150 O 161 -2.248 PHE 22.113 55.948 1.000 20.38 ANISOU 1150 O PHE 161 1981 3291 2473 -190 -191 - 72 MOTA 1151 CB PHE 161 -0.683 54.862 1.000 19.76 24.431 ANISOU 1151 CB PHE 161 2065 1903 3540 167 355 - 198 ATOM 1152 CG 161 -0.379 PHE 25.259 56.109 1.000 23.61 ANISOU 1152 CG PHE 161 3026 1905 4041 836 -59 -591 MOTA 1153 CD1 PHE 161 -1.194 25.304 57.228 1.000 28.25 ANISOU 1153 CD1 PHE 161 3992 2474 4268 1077 369 -1253 1154 CD2 PHE ATOM 161 0.807 56.141 1.000 26.62 25.978 ANISOU 1154 CD2 PHE 161 4015 2483 -130 -927 -106 3616 ATOM 1155 CE1 PHE 161 -0.850 25.992 58.383 1.000 35.29 ANISOU 1155 CE1 PHE 161 6873 2097 1538 -135 - 1399 4437 1156 CE2 PHE ATOM 161 1.153 26.723 57.258 1.000 33.63 ANISOU 1156 CE2 PHE 161 4643 3240 4894 1263 -2085 -1268 MOTA 1157 CZ 161 0.320 PHE 26.726 58.363 1.000 36.44 ANISOU 1157 CZ PHE 161 6071 4282 3493 1455 -2477 -1044 ATOM 1158 N 162 -0.358 ARG 21.767 57.130 1.000 17.59 ANISOU 1158 N ARG 162 2095 2103 2487 -118 -135 - 69 1159 CA ARG MOTA 162 -1.072 21.078 58.199 1.000 18.27 ANISOU 1159 CA ARG 162 2769 2414 1758 178 - 378 6

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						- 51 -			
ATOM	1160	С	ARG	162	-0.880	21.758	E0	1 000	20 16
ANISOU	1160				_	· -			20.16
			ARG		2110	3341	2210	-36	41 - 960
ATOM	1161	O	ARG	162	0.217	22.160	59.893	1.000	19.61
ANISOU	1161	0	ARG	162	2257	2993	2201	-194	
ATOM	1162		ARG						
					-0.580	19.640	58.356	1.000	20.81
ANISOU	1162		ARG	162	2958	2275	2675	-129	6 - 169
ATOM	1163	CG	ARG	162	-0.843	18.724			19.90
ANISOU	1163		ARG						
					3044	2073	2443	-112	254 - 38
ATOM	1164		ARG	162	-0.182	17.383	57.393	1.000	28.02
ANISOU	1164	CD	ARG	162	5599	2038	3010	381	-14 114
ATOM	1165	ME	ARG		-0.369	16.420			
ANISOU	1165						56.326	T.000	27.74
			ARG		4151	2294	4097	555	-687 -434
ATOM	1166	CZ	ARG	162	-1.278	15.445	56.370	1 000	31.11
ANISOU	1166	CZ	ARG	162	2560	3729	5531		
ATOM	1167				-2.092		· —	470	-350 -1152
						15.324	57.403	1.000	42.97
ANISOU	1167			162	3475	5906	6946	-579	1019 - 2492
ATOM	1168	NH2	ARG	162	-1.329	14.603	55.353		29.64
ANISOU	1168	NH2	ARG		3066	2738	_		
ATOM	1169						5458	120	-143 - 708
			TYR		-1.956	21.780	60.311	1.000	19.52
ANISOU	1169		TYR	163	2394	2901	2120	147	263 - 763
ATOM	1170	CA	TYR	163	-1.943	22.102	61.732		22.74
ANISOU	1170		TYR		3312				
ATOM						3107	2219	369	302 - 878
	1171	_	TYR		-2.037	20.800	62.536	1.000	24.20
ANISOU	1171	C	TYR	163	2802	3901	2492	-222	253 -189
ATOM	1172	0	TYR		-2.992	20.049	62.274		
ANISOU	1172		TYR						28.02
					2305	4409	3934	-202	-126 3 9 9
ATOM	1173		TYR	163	-3.198	22.912	62.114	1.000	28.98
ANISOU	1173	CB	TYR	163	3861	3231	3920	267	1196 - 1783
ATOM	1174	CG	TYR		-3.342	22.997			
ANISOU	1174						63.623	1.000	25.58
			TYR		2572	3382	3767	543	749 -1204
ATOM	1175			163	-2.458	23.826	64.319	1.000	37.32
ANISOU	1175	CD1	TYŔ	163	3654	6112	4413	-759	884 -2373
ATOM	1176				-4.315	22.333			
ANISOU							64.345		29.13
	1176				2622	3994	4452	749	1084 - 769
ATOM	1177			163	-2.546	23.966	65.702	1.000	38.28
ANISOU	1177	CE1	TYR	163	2905	7138	4503	-454	987 -2740
ATOM	1178				-4.396	22.431			
ANISOU	1178						65.726		
					3220	6336	4640	-273	1997 - 1618
ATOM	1179		TYR	163	-3.500	23.250	66.393	1.000	49.85
ANISOU	1179	CZ	TYR	163	5272	8795	4872		1593 - 2223
ATOM	1180		TYR		-3.595	23.365			
ANISOU	1180						67.768		
			TYR		5246	7368	4413	-222	270 - 496
ATOM	1181		PHE	164	-1.098	20.651	63.448	1.000	24.84
ANISOU	1181	N	PHE	164	2905	3368	3164	-89	-125 - 361
ATOM	1182		PHE		-1.045	19.532			
ANISOU	1182						64.370		28.14
			PHE		3538	3957	3195	223	-163 - 30
ATOM	1183	C	PHE	164	-1.360	20.003	65.787	1.000	26.67
ANISOU	1183	C	PHE	164	2964	3937	3234		-194 - 257
ATOM	1184	Ō	PHE		-0.540				·
						20.730			31.26
ANISOU		-	PHE	164	3119	4888	3869	-959	-260 - 519
ATOM	1185		PHE	164	0.347	18.881	64.396	1 000	27 86
ANISOU	1185	CB	PHE	164	3423	3725			
ATOM	1186						7470	/ O ~ I :	99 - 32
				104	0.744	18.301			
	1186				2914	3474	3785	-598	74 - 275
ATOM	1187	CD1	PHE	164	1.435	19.093			
ANISOU	1187				2827	3836			
ATOM	1188								-615 7 1 1
					0.414	16.996			
	1188				4365	2808	4698	349	-298 - 96
ATOM	1189	CE1	PHE	164	1.787	18.609			
ANISOU	1189	CF1	PHF		3609	5052	2771		
ATOM	1190								-1030 641
	~ 1 2 0	کیڈ پ	THE	104	0.786	16.501	01.4/5	T.000	38.25

				- 52 -	
ANISO			164 6659	4077	3797 -740 -1363 -612
ATOM	1191 CZ		164 1.494	17.298	
ANISO		PHE	164 3189	5078	4172 712 -944 - 385
ATOM	1192 N	PRO	165 -2.469	19.609	66.379 1.000 30.62
ANISOU		PRO	165 3876	4009	3751 -1371 344 -508
ATOM	1193 CA		165 -2.670	19.813	67.809 1.000 33.09
ANISOU			165 3299	5764	3510 -190 80 2 3 6
ATOM	1194 C	PRO	165 -1.459	19.408	68.638 1.000 36.32
ATOM	J 1194 C	PRO	165 3538	5745	4518 664 -191 - 234
ANISOU	1195 O 1 1195 O		165 -0.776	18.428	68.371 1.000 32.94
ATOM	1196 CB	PRO	165 4268	4761	3487 220 501 387
ANISOU		PRO PRO	165 -3.882	18.929	68.123 1.000 38.44
ATOM	1197 CG	PRO	165 3807	6924	3873 -765 271 827
ANISOU		PRO	165 -4.635 165 2595	18.842	66.845 1.000 35.82
ATOM	1198 CD	PRO	165 -3.690	7020	3995 5 688 - 828
ANISOU		PRO	165 3192	19.130 5919	65.710 1.000 33.90
ATOM	1199 N	LEU	178 7.727	7.453	3770 -1149 194 169
ANISOU	1199 N	LEU	178 12297	5376	68.180 1.000 64.52 6843 278 -218 3721
ATOM	1200 CA	LEU	178 7.629	8.260	
ANISOU		LEU	178 10557	2730	
ATOM	1201 C	LEU	178 6.159	8.539	3168 -984 -2821 -135 66.662 1.000 47.36
ANISOU		LEU	178 9239	3530	5225 -2598 -1186 1204
ATOM ANISOU	1202 0	LEU	178 5.314	7.659	66.796 1.000 56.53
ATOM	1202 O 1203 CB	LEU	178 11777	5626	4076 -4835 1265 -602
ANISOU		LEU	178 8.222	7.582	65.746 1.000 55.55
ATOM	1203 CB	LEU LEU	178 11470	3734	5902 -1314 -1197 -1822
ANISOU	1204 CG	LEU	178 <sup>3</sup> 9.662 178 10812	7.092	65.774 1.000 62.34
ATOM	1205 CD1	LEU	178 9.916	5116	7760 -1971 194 -443
ANISOU	1205 CD1	LEU	178 9626	6.185 4989	64.579 1.000 54.23
ATOM	1206 CD2	LEU	178 10.633	8.264	5988 1878 -3799 511
ANISOU	1206 CD2	LEU	178 11265	3454	65.773 1.000 66.44
ATOM	1207 N	ARG	179 5.879	9.751	10526 -1170 4090 -516 66.192 1.000 52.90
ANISOU		ARG	179 7853	3826	8421 102 1230 1 0 3 1
ATOM	1208 CA	ARG	179 4.495	10.033	65.807 1.000 51.26
ANISOU ATOM	1208 CA	ARG	179 7235	4820	7421 -229 1890 - 383
ANISOU	1209 C 1209 C	ARG	179 4.242	9.563	64.383 1.000 55.25
ATOM	1210 0	ARG	179 7178	6083	7731 -946 2260 -1134
	1210 0	ARG	179 3.120	9.211	64.021 1.000 58.51
ATOM	1211 CB	ARG ARG	179 7036 179 4.180	7628	7565 -1820 3675 -2851
	1211 CB	ARG	179 4.180 179 6600	11.512	66.040 1.000 41.49
ATOM	1212 CG	ARG	179 3.293	4448	4716 -155 1916 1137
ANISOU	1212 CG	ARG	179 6120	11.700 5908	1000 10.15
ATOM	1213 CD	ARG	179 1.888	12.059	4367 90 1338 5 3 0 66.833 1.000 47.63
ANISOU	1213 CD	ARG	179 6180	7453	4.463
ATOM	1214 NE	ARG	179 1.459	13.367	4463 195 860 - 531 67.269 1.000 52.00
ANISOU	1214 NE	ARG	179 7384	7834	4539 1669 -1168 -538
ATOM	1215 CZ	ARG	179 1.322	14.470	
ATOM	1215 CZ	ARG	179 10838	8000	5788 1457 -1107 6 3
	1216 NH1 1216 NH1	ARG	179 1.637	14.518	65.268 1.000 59.74
ATOM	1216 NH1 1217 NH2	AKG	1/9 9535	8090	5074 3628 -2691 445
	1217 NH2	ARG	179 0.907	15.606	67.117 1.000 65.83
ATOM	1218 N	MET	179 10451 180 5.304	9083	5478 4171 -776 1200
		MET	180 5383	9.501	63.589 1.000 43.96
MOTA	1219 CA	MET	180 5.264	3769 9.035	7550 705 852 -1245
	1219 CA	MET	180 2356		62.210 1.000 40.44 7543 -398 574 -1482
ATOM	1220 C	MET	180 6.552		
ANISOU	1220 C	MET	180 2731	6220	
					7733 18 320 - 2324

					00			
ATOM	1221	$\circ$	MET	180 7.629	8.679	62 227	1 000	20 46
						62.327		39.46
ANISOU	1221		MET	180 2377	5064	7554	-395	906 - 912
ATOM	1222	CB	MET	180 5.129	10.189	61.219	1.000	49.84
ANISOU	1222	CB	MET	180 2749	7966			
						8223	-452	-1114 7 2
ATOM	1223	CG	MET	180 5.339	9.818	59.757	1.000	62.58
ANISOU	1223	CG	MET	180 7280	8911	7587	-2331	-3353 -505
ATOM	1224							
			MET	180 4.622	11.015	58.608	1.000	74.24
ANISOU	1224	SD	MET	180 7480	13510	7216	4918	-262 - 905
ATOM	1225	CE	MET	180 4.501	10.037		1.000	79.59
ANISOU	1225							
			MET	180 6119	20000	4120	-1978	1874 - 912
ATOM	1226	N	ALA	181 6.376	7.112	61.275	1.000	37.44
ANISOU	1226	N	ALA	181 3523	5646	5055	-271	
ATOM	1227							882 -1132
			ALA	181 7.407	6.140		1.000	37.40
ANISOU	1227	CA	ALA	181 3980	3980	6250	-625	2048 4 6 1
ATOM	1228	С	ALA	181 8.287	6.591	59.837		31.49
ANISOU	1228		ALA					
				181 2975	3842	5149	-32	920 956
ATOM	1229	O	ALA	181 7.834	7.393	58.997	1.000	30.77
ANISOU	1229	0	ALA	181 2903	4021	4765	197	-98 164
ATOM	1230		ALA	181 6.727				•
					4.817		1.000	42.66
ANISOU	1230	CB	ALA	181 4105	4284	7820	-1023	1629 5 5 7
ATOM	1231	N	PRO	182 9.541	6.137	59.840	1.000	24.52
ANISOU	1231		PRO	182 2782				
					4237	2296	-240	-76 320
ATOM	1232		PRO	182 10.442	6.667	58.820	1.000	20.55
ANISOU	1232	CA	PRO	182 2612	2870	2326	-335	-117 - 65
ATOM	1233	$\subset$	PRO	182 9.958	6.402			
						57.408		19.31
ANISOU	1233		PRO	182 2609	2491	2236	-391	48 - 86
ATOM	1234	0	PRO	182 9.448	5.326	57.080	1.000	21.68
ANISOU	1234	Ο	PRO	182=2991	2486	2759	-440	-340 - 55
ATOM	1235		PRO	182 11.768	5.939	59.047	1.000	24.98
ANISOU	1235	CB	PRO	182 2589	3860	3042	-170	-286 1 5 3
ATOM	1236	CG	PRO	182 11.681	5.351	60.393		28.42
ANISOU	1236		PRO					
				182 3352	3582	3863	656	321 1038
ATOM	1237		PRO	182 10.215	5.210	60.747	1.000	32.21
ANISOU	1237	CD	PRO	182 3333	4905	4000	-826	-390 1785
ATOM	1238		HIS	183 10.111				
					7.414	56.561		19.27
ANISOU	1238		HIS	183 2131	2658	2533	-274	-204 1 7 6
ATOM	1239	CA	HIS	183 9.757	7.306	55.144	1.000	18.01
ANISOU	1239	CA	HIS	183 1882	2311	2652	-341	-455 3 4 6
ATOM	1240							
			HIS	183 10.749	8.124	54.337		15.74
ANISOU	1240		HIS	183 1964	1560	2456	-75	-352 1 2 8
ATOM	1241	0	HIS	183 11.355	9.061	54.868	1.000	18.14
ANISOU	1241	$\cap$	HIS	183 2297	2093	2504	-509	-127 - 135
ATOM								
	1242		HIS	183 8.338	7.781	54.835	1.000	18.66
ANISOU	1242	CB	HIS	183 1970	2173	2945	-136	-243 3 7 1
ATOM	1243	CG	HIS	183 8.089	9.120	55.447		26.67
ANISOU	1243		HIS	183 3100				
					2751	4281	262	222 - 306
ATOM	1244			183 7.884	9.362	56.800	1.000	35.36
ANISOU	1244	ND1	HIS	183 4432	4078	4926	-1190	1466 - 1454
ATOM	1245	CD2	HTS	183 8.051	10.311			33.00
				183 4117	2522	5898	1687	-677 -173
ATOM	1246	CEI	HIS	183 7.739	10.658	56.980	1.000	35.91
ANISOU	1246	CE1	HTS	183 2611	4468	6565		-625 -2616 .
ATOM	1247							
				183 7.829	11.251			
	1247		HIS	183 4375	3417	7614	1821	-1013 - 1590
ATOM	1248	N	TYR	184 10.890	7.778	53.061		15.68
ANISOU	1248		TYR	184 1973				
					1551	2434		-470 1 0 7
ATOM	1249		TYR	184 11:605	8.685	52.152	1.000	14.81
ANISOU	1249	CA	TYR	184 1798	1392	2438	147	-312 1 4 5
ATOM	1250	C	TYR	184 10.572		51.169		
ANISOU	1250	_			<del>-</del>			
			TYR	184 1656	1449	2416		-399 9 8
ATOM	1251	U	TYR	184 9.468	8.728	51.045	1.000	15.83

		<b>~</b> 4			
ANISOU 1251 O ATOM 1252 CB ANISOU 1253 CG ANISOU 1253 CG ANISOU 1253 CG ATOM 1254 CD1 ANISOU 1254 CD1 ATOM 1255 CD2 ANISOU 1255 CD2 ANISOU 1255 CE1 ANISOU 1256 CE1 ATOM 1257 CE2 ANISOU 1257 CE2 ANISOU 1258 CZ ANISOU 1259 OH ANISOU 1259 OH ANISOU 1259 OH	TYR 184 154 TYR 184 12. TYR 184 172 TYR 184 11. TYR 184 169 TYR 184 12.	.699       8.004         .36       1323         .383       6.785         .313       1313         .200       5.540         .329       6.836         .329       6.836         .3962       4.396         .3962       4.396         .130       5.661         .1776       1736         .915       4.449         .55       1736         .682       3.325	2586 51.185 3021 49.165 2552 50.442 2992 48.447 2540 49.083 3014	-103 -448 1 5 1.000 15.66 69 -366 -16 1.000 14.85 109 -567 4 1.000 15.49 -29 -575 1 9 1.000 15.89 55 -27 - 64 1.000 15.61 229 -137 1 1 1.000 17.52 4 83 - 9 0 1.000 16.96 -156 -480 3 4 1.000 18.81 260 -277 - 3	8 3 0 3
ANISOU 1260 N ATOM 1261 CA	ASP 185 10. ASP 185 151	1599	2338	1.000 14.36 87 -225 276	
ANISOU 1261 CA	ASP 185 10. ASP 185 187	75 1322	2078	1.000 13.88 $141 -364 - 4$	2
ATOM 1262 C ANISOU 1262 C	ASP 185 118		2211	1.000 12.57 $-160 -77 -1$	3 0
ATOM 1263 O ANISOU 1263 O	ASP 185 11. ASP 185 117	77 1637	47.824 2559	1.000 14.14 -135 146 14	0
ATOM 1264 CB ANISOU 1264 CB	ASP 185 10. ASP 185 187	79 1293	49.580 2517	1.000 14.97 121 -186 -1	5 9
ATOM 1265 CG ANISOU 1265 CG	ASP 185 9.7 ASP 185 268		50.830 2351	1.000 17.61 232 -13 -1	7 2
ATOM 1266 OD1 ANISOU 1266 OD1				1.000 23.69 443 -302 5 2	
	ASP 185 9.1	174 14.257		1.000 24.32	
ATOM 1268 N ANISOU 1268 N	LEU 186 9.1	141 10.465	47.382		
ATOM 1269 CA	LEU 186 127 LEU 186 9.1	169 10.091	2126 45.986	-117 -117 -1 1.000 12.92	17
ANISOU 1269 CA ATOM 1270 C	LEU 186 153 LEU 186 9.1		2150 45.052	-331 $-84$ $-1$ $1.000$ $14.12$	7 5
ANISOU 1270 C ATOM 1271 O	LEU 186 173 LEU 186 8.9	30 1307	2330	-93 -165 5 5 1 . 000 20 . 12	5 .
ANISOU 1271 O ATOM 1272 CB	LEU 186 372	21 1643	2280	-423 99 9 2	
ANISOU 1272 CB	LEU 186 8.0 LEU 186 150	09 1310	45.609 2393	1.000 13.72 -270 -375 -	6
ATOM 1273 CG ANISOU 1273 CG	LEU 186 8.0 LEU 186 154	_ <del>_</del>	46.438 3361	1.000 15.92 -145 -307 16	5 8
ATOM 1274 CD1 ANISOU 1274 CD1		929 6.908		1.000 19.36 -700 -209 3 9	
ATOM 1275 CD2 ANISOU 1275 CD2	LEU 186 9.:	369 7.115	46.341	1.000 18.32	
ATOM 1276 N ANISOU 1276 N	SER 187 9.3	286 12.494		200 -432 1 7 1.000 13.60	
ATOM 1277 CA	SER 187 133 SER 187 9.3	388 13.734	2608 44.826	-26 -95 13 1.000 13.22	7
ANISOU 1277 CA ATOM 1278 C	SER 187 148 SER 187 10			-54 -68 2 1.000 12.79	9
ANISOU 1278 C ATOM 1279 O	SER 187 148 SER 187 11		2192	-17 -114 - 9 1.000 14.50	) 0
ANISOU 1279 O ATOM 1280 CB	SER 187 15: SER 187 9.	32 1257	2720	76 -224 -11 1.000 12.87	3
ANISOU 1280 CB ATOM 1281 OG	SER 187 14	63 1282	2147	164 -154 9	8
ANISOU 1281 OG	SER 187 10 SER 187 15		2015	1.000 13.22 -34 -143 22	2 4

- 55 -188 10.898 14.844 MOTA 1282 N MET 43.292 1.000 13.44 ANISOU 1282 N MET 188 1552 1334 2221 -64 -34 -26MOTA 1283 CA MET 188 12.215 15.380 42.878 1.000 12.11 ANISOU 1283 CA MET 188 1508 1261 1833 29 -60 - 61 1284 C MOTA MET 188 12.853 44.104 1.000 12.78 16.022 ANISOU 1284 C MET 1156 188 1563 2136 167 -311 - 42 ATOM 1285 0 MET 188 13.896 44.600 1.000 13.40 15.550 ANISOU 1285 O MET 188 1408 1390 2294 116 -264 - 26 ATOM MET 188 12.038 1286 CB 16.300 41.667 1.000 13.66 ANISOU 1286 CB MET 188 1565 1501 2123 44 -161 207 1287 CG MET 188 13.296 17.095 41.315 1.000 14.05 ATOM ANISOU 1287 CG MET 188 1697 1595 66 150 1 3 3 2046 MET 188 14.600 MOTA 1288 SD 15.971 40.752 1.000 14.96 MET ANISOU 1288 SD 188 1565 1591 2529 109 -81 110. 1289 CE 188 16.005 17.102 ATOM MET 40.686 1.000 17.74 ANISOU 1289 CE MET 188 1852 2032 2855 -242 505 121 189 12.244 17.112 44.616 1.000 12.62 ATOM 1290 N VAL ANISOU 1290 N VAL 189 1586 1203 2007 103 -147 - 1341291 CA 189 12.565 17.671 45.918 1.000 12.60 ATOM VAL ANISOU 1291 CA VAL 189 1412 1438 1937 -228 -11 -441292 C 189 11.285 17.968 46.679 1.000 11.71 ATOM VAL ANISOU 1292 C VAL 189 1328 1294 1825 -170 -171 - 4 9 1293 0 189 10.227 18.099 46.050 1.000 12.56 ATOM VAL ANISOU 1293 O VAL 189 1446 1291 21 -320 - 49 2036 ATOM 189 13.440 18.955 45.856 1.000 12.95 1294 CB VAL ANISOU 1294 CB VAL 189 1150 1517 2252 -174 -205 9 4 1295 CG1 VAL ATOM 189 14.778 45.167 1.000 15.54 18.637 ANISOU 1295 CG1 VAL 189 1376 2094 2437 -140 161 9 1 1296 CG2 VAL 189 12.730 20.056 45.082 1.000 15.00 ATOM ANISOU 1296 CG2 VAL 189 1763 1391 -130 -483 8 1 2547 ATOM 190 11.425 18.067 1297 N THR 47.984 1.000 12.18 190 1445 ANISOU 1297 N THR 1422 1760 -109 -130 1 0 1298 CA ATOM 190 10.353 18.454 THR 48.897 1.000 11.98 ANISOU 1298 CA THR 190 1292 1356 1903 -57 -221 -151 ATOM 1299 C THR 190 10.879 19.630 49.710 1.000 12.47 ANISOU 1299 C THR 190 1178 1436 2124 -297 -232 -32 1300 0 190 11.959 19.523 ATOM THR 50.320 1.000 15.06 ANISOU 1300 O THR 190 1424 1767 2531 46 -571 -446 ATOM 1301 CB THR 190 9.913 17.297 49.808 1.000 13.16 ANISOU 1301 CB 190 1509 THR 1605 1886 -168 80 -121 ATOM 1302 OG1 THR 190 9.481 16.201 48.993 1.000 14.47 ANISOU 1302 OG1 THR 190 1693 1469 2334 -100 -25 -1941303 CG2 THR ATOM 190 8.778 17.723 50.734 1.000 14.79 ANISOU 1303 CG2 THR 190 1696 1510 2415 73 258 - 89 ATOM 1304 N 191 10.148 20.724 LEU 49.732 1.000 12.97 ANISOU 1304 N 191 1329 LEU 1449 2149 23 -21 - 286 1305 CA LEU MOTA 191 10.511 21.908 50.526 1.000 13.75 ANISOU 1305 CA LEU 191 1543 1442 78 -206 - 301 2238 ATOM 1306 C LEU 191 9.603 21.964 51.763 1.000 14.47 ANISOU 1306 C LEU 191 1543 2265 83 -179 -412 . 1689 1307 0 ATOM LEU 191 8.370 21.868 51.645 1.000 16.58 ANISOU 1307 O 191 1517 LEU 2486 219 -176 - 725 2297 1308 CB ATOM 191 10.398 23.212 LEU 49.722 1.000 15.37 ANISOU 1308 CB LEU 191 1717 1444 2680 58 - 106 - 189 1309 CG LEU ATOM 191 11.705 -23.578 48.973 1.000 16.10 'ANISOU 1309 CG LEU 191 1747 1688 -128 -113 -135 2680 1310 CD1 LEU ATOM 191 12.069 22.565 47.906 1.000 16.67 ANISOU 1310 CD1 LEU 191 2034 2093 2209 -23 -64 1 9 1311 CD2 LEU ATOM 191 11.570 24.959 48.350 1.000 18.53 ANISOU 1311 CD2 LEU 191 2297 1906 2837 -345 -437 1 4 8 ATOM 1312 N 192 10.199 22.148 ILE 52.946 1.000 15.36

- 56 -

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ANISOU 1312 N
                 ILE
                      192 1479
                                  2152
                                          2204
                                                        -165 - 164
                                                  -47
       1313 CA
MOTA
                ILE
                      192 9.417
                                  22.162
                                          54.194 1.000 15.13
ANISOU 1313 CA
                ILE
                      192 1456
                                  2043
                                                        -173 -280
                                          2251
                                                  -304
ATOM
       1314 C
                ILE
                      192 9.692
                                  23.423
                                          55.010 1.000 15.58
ANISOU 1314 C
                ILE
                      192 1696
                                  1973
                                          2251
                                                  -199
                                                        -254 - 226
ATOM
       1315 0
                ILE
                      192 10.836
                                  23.691
                                          55.381 1.000 17.20
ANISOU 1315 O
                      192 1856
                ILE
                                  2449
                                          2229
                                                  -307
                                                        -341 -574
       1316 CB
MOTA
                ILE
                      192 9.722
                                          55.040 1.000 17.03
                                  20.920
ANISOU 1316 CB
                ILE
                      192 2246
                                  1958
                                          2266
                                                  -52
                                                        325 - 303
       1317 CG1 ILE
                      192 9.454
MOTA
                                          54.317 1.000 19.80
                                  19.596
ANISOU 1317 CG1 ILE
                                  2010
                      192 3040
                                          2473
                                                        128 - 382
                                                  -71
       1318 CG2 ILE
                      192 8.995
MOTA
                                          56.403 1.000 18.14
                                  20.967
ANISOU 1318 CG2 ILE
                                  2354
                      192 2278
                                          2262
                                                  229
                                                        290 - 258
       1319 CD1 ILE
                      192 9.420
ATOM
                                          55.235 1.000 31.57
                                  18.387
ANISOU 1319 CD1 ILE
                      192 4658
                                  2114
                                          5222
                                                  -398
                                                        -1094 765
       1320 N
ATOM
                GLN
                      193 8.625
                                          55.249 1.000 17.04
                                  24.172
ANISOU 1320 N
                GLN
                      193 2042
                                  2185
                                          2248
                                                 112
                                                        -388 - 301
       1321 CA
MOTA
               GLN
                      193 8.680
                                          56.201 1.000 17.70
                                  25.291
ANISOU 1321 CA
                GLN
                      193 1737
                                  2167
                                          2824
                                                 -204
                                                        -186 - 559
       1322 C
ATOM
                GLN
                      193.7.898
                                  24.869
                                          57.443 1.000 19.67
ANISOU 1322 C
                GLN
                      193 1882
                                          2969
                                  2624
                                                  -232
                                                        211 - 840
       1323 0
ATOM
                GLN
                      193 7.082
                                  23.942
                                          57.426 1.000 26.60
ANISOU 1323 O
                      193 2066
                GLN
                                  3843
                                                        -110 6 2
                                          4197
                                                  -965
ATOM
       1324 CB
                GLN
                      193 8.129
                                          55.643 1.000 23.74
                                  26.598
ANISOU 1324 CB
                GLN
                      193 3070
                                  2388
                                          3561
                                                 500
                                                        -98 - 514
ATOM
       1325 CG
                GLN
                      193 8.913
                                          54.559 1.000 28.26
                                  27.304
ANISOU 1325 CG
                GLN
                      193 4664
                                  2384
                                          3689
                                                  656
                                                        209 0
       1326 CD
ATOM
                      19328.338
                GLN
                                  28.665
                                          54.156 1.000 26.30
ANISOU 1326 CD
                GLN
                      193 2868
                                  2943
                                          4181
                                                 791
                                                        3
                                                           1 1 1
       1327 OE1 GLN
                      193 7.193
ATOM
                                  28.695
                                          53.688 1.000 45.31
ANISOU 1327 OE1 GLN
                      193 2826
                                  7147
                                          7241
                                                  -51
                                                        -616 3173
       1328 NE2 GLN
ATOM
                      193 9.080
                                  29.748
                                          54.345 1.000 30.44
ANISOU 1328 NE2 GLN
                      193 3609
                                  2588
                                                  418
                                          5368
                                                        1259 6 9 2
       1329 N
ATOM
                GLN
                      194 8.241
                                          58.645 1.000 22.04
                                  25.259
ANISOU 1329 N
                GLN
                      194 2926
                                  2758
                                          2690
                                                 303
                                                        -368 - 83
ATOM
       1330 CA
               GLN
                      194 7.569
                                  24.793
                                          59.847 1.000 22.68
ANISOU 1330 CA
                GLN
                      194 3144
                                  2617
                                         2855
                                                  82 -230 -150
       1331 C
ATOM
                GLN
                      194 7.275
                                          60.663 1.000 22.19
                                  26.054
ANISOU 1331 C
                GLN
                                  2768
                      194 2809
                                          2856
                                                 117
                                                        -396 - 320
ATOM
       1332 0
                GLN
                      194 7.889
                                          60.418 1.000 25.26
                                  27.100
                GLN
ANISOU 1332 O
                      194 4041
                                  2877
                                          2679
                                                  -313
                                                        -21 - 411
ATOM
       1333 CB
                GLN
                                  23.943
                      194 8.467
                                          60.739 1.000 29.21
ANISOU 1333 CB
                GLN
                      194 4493
                                  2707
                                          3899
                                                  477
                                                        -50 939
ATOM
       1334 CG
                GLN
                      194 9.105
                                  22.735
                                          60.083 1.000 28.80
ANISOU 1334 CG
                GLN
                      194 3108
                                  3530
                                          4305
                                                  576
                                                        -121494
ATOM
       1335 CD
               GLN
                      194 10.296
                                          60.962 1.000 31.97
                                  22.332
ANISOU 1335 CD GLN
                      194 2961
                                  5384
                                          3800
                                                  824
                                                        359 1075
       1336 OE1 GLN
ATOM
                      194 11.421
                                          60.474 1.000 27.28
                                  22.325
ANISOU 1336 OE1 GLN
                      194 2781
                                  4189
                                          3397
                                                  118
                                                        133 - 249
       1337 NE2 GLN
ATOM
                      194 9.998
                                          62.232 1.000 29.82
                                  22.100
ANISOU 1337 NE2 GLN
                      194 3540
                                  3958
                                          3832
                                                  989
                                                        645 800
       1338 N
ATOM
                THR
                      195 6.419
                                  25.891
                                          61.658 1.000 23.30
ANISOU 1338 N
                THR
                      195 2407
                                  3058
                                          3387
                                                  -211
                                                        -235 -720
ATOM
       1339 CA
                THR
                      195 6.476
                                          62.768 1.000 27.14
                                  26.833
ANISOU 1339 CA
                THR
                      195 3459
                                  3544
                                          3308
                                                  25 -50 -890
ATOM
       1340 C
                      195 6.933
                                  25.997
                THR
                                          63.958 1.000 26.11
ANISOU 1340 C
                THR
                                  2829
                      195 3825
                                          3268
                                                  558
                                                        19 -1247
ATOM
       1341 0
                THR
                      195 6.639
                                          63.994 1.000 28.17
                                  24.815
ANISOU 1341 O
                THR
                      195 2973
                                  2916
                                           4815
                                                        171 -1030
                                                  481
ATOM
       1342 CB
                 THR
                      195 5.149
                                          63.069 1.000 25.87
                                  27.534
ANISOU 1342 CB
                 THR
                      195 3428
                                  2849
                                           3551
                                                  -16
                                                        -592 -1137
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- 57 -MOTA 1343 OG1 THR 26.550 195 4.111 63.196 1.000 25.45 ANISOU 1343 OG1 THR 195 3427 3101 3141 -9 **-117** - 750 1344 CG2 THR MOTA 195 4.788 28.396 61.847 1.000 31.31 ANISOU 1344 CG2 THR 195 4965 2552 4380 274 -70 -409 ATOM 1345 N PRO 196 7.604 64.923 1.000 30.84 26.587 ANISOU 1345 N 196 5225 PRO 3191 3300 785 -517 - 15421346 CA MOTA 196 8.101 66.065 1.000 28.50 PRO 25.823 ANISOU 1346 CA PRO 196 3113 3700 -279 -441 -646 4016 1347 C MOTA PRO 196 7.018 25.534 67.096 1.000 28.97 ANISOU 1347 C PRO 196 3581 3326 42 113 -1381 4102 196 6.002 ATOM 1348 0 PRO 26.229 67.192 1.000 32.32 ANISOU 1348 O PRO 196 4146 4649 3485 901 -180 -1658 ATOM PRO 1349 CB 196 9.094 26.816 66.694 1.000 29.72 ANISOU 1349 CB PRO 196 3888 3292 -285 -353 -1072 4111 1350 CG ATOM 196 8.533 PRO 66.364 1.000 34.87 28.174 ANISOU 1350 CG PRO 196 6285 3575 3390 421 -1326 -1332 1351 CD PRO MOTA 196 7.897 28.035 65.012 1.000 33.20 ANISOU 1351 CD PRO 196 6407 3606 -598 -494 -1031 2600 1352 N ATOM 197 7.289 CYS 24.533 67.919 1.000 26.96 ANISOU 1352 N 197 2739 CYS 3465 -113 85 -1227 4038 1353 CA ATOM CYS 197 6.519 24.289 69.126 1.000 31.73 ANISOU 1353 CA CYS 197 3979 4543 3533 -39 721 -1726 1354 C ATOM 197 6.803 CYS 70.124 1.000 35.58 25.412 ANISOU 1354 C CYS 197 4213 4819 4486 -480 1126 -2282 ATOM 1355 0 CYS 197 7.917 70.175 1.000 31.34 25.939 ANISOU 1355 O CYS 197 3817 4845 3246 36 - 383 - 992 197 6.940 ATOM 1356 CB CYS 22.962 69.767 1.000 35.79 ANISOU 1356 CB CYS 197 5913 4705 2980 284 1566 - 1423 1357 SG ATOM CYS 197 6.553 21.535 68.741 1.000 28.53 197 3605 ANISOU 1357 SG CYS 3009 4224 50 -5 - 452 1358 N ATOM ALA 70.866 1.000 37.27 198 5.771 25.791 ANISOU 1358 N ALA 198 5038 4984 4139 -421 1647 - 2070 1359 CA ATOM ALA 198 5.983 26.811 71.888 1.000 35.91 ANISOU 1359 CA ALA198 6273 4144 3230 910 522 - 12301360 C ATOM ALA 198 6.993 72.921 1.000 44.30 26.328 ANISOU 1360 C ALA 198 5998 6138 4696 -193 -199 3 3 1361 0 ATOM ALA 198 7.759 73.457 1.000 42.85 27.127 ANISOU 1361 O ALA 198 5209 6328 4742 7 490 - 555 1362 CB 198 4.671 ATOM ALA 27.231 72.532 1.000 41.70 ANISOU 1362 CB ALA 5697 2557 198 7588 2355 1068 - 721 ATOM 1363 N ASN 199 7.036 25.036 73.225 1.000 34.93 ANISOU 1363 N 199 4027 ASN 5975 3270 805 167 -621 ATOM 1364 CA ASN 199 7.969 74.264 1.000 33.58 24.578 ANISOU 1364 CA ASN 199 3643 6167 2950 -670 -265 -808 1365 C ATOM ASN 199 9.352 24.262 73.718 1.000 31.53 ANISOU 1365 C ASN 199 4077 5048 2853 -420 - 855384 MOTA 1366 0 ASN 199 10.153 23.667 74.467 1.000 36.33 ANISOU 1366 O 199 4223 ASN 5624 3957 -403 -1305 -126 ATOM 1367 CB ASN 199 7.441 23.308 74.929 1.000 36.38 ANISOU 1367 CB ASN 199 4533 5029 4262 859 584 - 522 ATOM 1368 CG ASN 199 7.198 22.180 73.952 1.000 31.28 ANISOU 1368 CG ASN 199 4030 2993 4863 882 202 178 1369 OD1 ASN ATOM 199 7.743 72.853 1.000 37.62 22.151 ANISOU 1369 OD1 ASN 199 4693 6272 3330 728 - 56 122 1370 ND2 ASN ATOM 199 6.393 74.314 1.000 36.42 21.190 ANISOU 1370 ND2 ASN 199 3508 1132 - 958 6251 -13 4078 1371 N ATOM GLY 200 9.616 24.569 72.449 1.000 30.93 ANISOU 1371 N GLY 200 4342 4232 3179 436 144 - 692 1372 CA GLY ATOM 24.304 71.866 1.000 35.26 200 10.920 ANISOU 1372 CA GLY 200 4430 4905 4060 -317 480 -2400 1373 C ATOM GLY 200 11.184 22.886 71.429 1.000 36.83

**-** 58 -ANISOU 1373 C GLY 200 4683 4375 4936 -360 1601 - 1460 ATOM 1374 0 GLY 22.566 200 12.257 70.897 1.000 32.71 ANISOU 1374 O GLY 200 3921 4072 4436 -377 752 -1400 201 10.264 ATOM 1375 N PHE 21.939 71.588 1.000 28.66 ANISOU 1375 N PHE 201 3813 4229 2847 145 463 - 326 ATOM 1376 CA PHE 201 10.491 71.106 1.000 27.55 20.575 ANISOU 1376 CA PHE 201 3190 4337 2943 -233 219 -672 201 10.752 MOTA 1377 C PHE 69.600 1.000 24.89 20.553 ANISOU 1377 C PHE 201 2943 3682 2832 190 -268 - 3791378 0 PHE - 201-9.994 ATOM 68.910 1.000 28.22 21.255 ANISOU 1378 O PHE 201 3583 3184 3957 10 -421 277 1379 CB PHE ATOM 19.729 201 9.250 71.413 1.000 30.46 ANISOU 1379 CB PHE 201 3153 4862 3560 -371 -40 - 731380 CG PHE 201 9.425 ATOM 71.027 1.000 34.89 18.262 ANISOU 1380 CG PHE 201 4015 4609 4632 -772 162 8 9 1381 CD1 PHE ATOM 201 10.395 17.472 71.605 1.000 31.18 ANISOU 1381 CD1 PHE 201 3436 4103 4310 -875 -93 -1105 1382 CD2 PHE 201 8.613 ATOM 17.681 70.078 1.000 28.84 ANISOU 1382 CD2 PHE 201 2979 4019 3960 329 612 - 1071383 CE1 PHE 201 10.564 ATOM 71.240 1.000 37.73 16.160 ANISOU 1383 CE1 PHE 201 6489 3608 4239 -1078 - 1475 - 5001384 CE2 PHE ATOM 201 8.761 69.679 1.000 31.78 16.363 ANISOU 1384 CE2 PHE 201 4327 3911 3838 652 250 119 MOTA 201 9.755 1385 CZ PHE 15.606 70.265 1.000 29.78 ANISOU 1385 CZ 201 3705 PHE 3397 4211 6 -638 -849 1386 N ATOM VAL 202 11.706 19.751 69.144 1.000 23.51 ANISOU 1386 N 202 2671 VAL 3392 -292 2868 -1 - 5781387 CA 202-11.969 ATOM VAL 67.706 1.000 26.37 19.626 202 3025 ANISOU 1387 CA VAL 4050 2946 -667 57 - 7241388 C MOTA VAL 202 11.423 18.283 67.198 1.000 22.75 ANISOU 1388 C VAL 202 2729 3348 2567 96 -120 ATOM 1389 0 VAL 202 11.880 67.541 1.000 28.71 17.190 ANISOU 1389 O VAL 202 3249 3799 3859 119 31 6 6 1 ATOM 1390 CB VAL 202 13.476 67.415 1.000 24.99 19.721 ANISOU 1390 CB VAL 202 3060 3427 3008 -278 283 152 1391 CG1 VAL ATOM 19.464 202 13.715 65.938 1.000 27.70 ANISOU 1391 CG1 VAL 202 4642 2577 3307 87 1014 1392 CG2 VAL 202 14.050 ATOM 21.071 67.823 1.000 26.80 ANISOU 1392 CG2 VAL 202 2826 3868 3487 -490 474 -398MOTA 1393 N 203 10.405 SER 66.333 1.000 24.10 18.402 ANISOU 1393 N SER 203 2194 3607 3356 -31 -179 - 528ATOM 1394 CA SER 203 9.634 17.231 65.940 1.000 23.70 ANISOU 1394 CA SER 203 2373 3584 3046 -290 308 -533 ATOM 1395 C 16.511 SER 203 10.168 64.710 1.000 21.28 ANISOU 1395 C 203 2173 SER 3041 2871 46 227 - 42ATOM 1396 O 203 10.159 SER 15.285 64.640 1.000 27.60 ANISOU 1396 O 203 4105 SER 3097 3284 -482 1010 - 249 1397 CB ATOM 203 8.148 SER 65.685 1.000 29.06 17.571 ANISOU 1397 CB SER 203 2251 3790 -180 203 - 2064 5001 ATOM 1398 OG SER 203 7.584 66.843 1.000 32.55 18.175 ANISOU 1398 OG SER 203 3840 4298 4231 920 1099 - 382ATOM 1399 N 204 10.688 LEU 17.233 63.724 1.000 22.46 ANISOU 1399 N 204 2476 3043 LEU 79 450 - 46 3013 ATOM 1400 CA LEU 204 11.166 62.544 1.000 20.26 16.530 ANISOU 1400 CA LEU 204 2200 2831 2667 45 - 18 - 15 ATOM 1401 C LEU 204 12.595 62.747 1.000 18.83 16.038 ANISOU 1401 C 204 2151 LEU 2477 2528 -75 60 - 1MOTA 1402 0 LEU 204 13.443 63.251 1.000 20.47 16.783 ANISOU 1402 O 204 2333 LEU 2386 3059 -303-195 4 0 4 ATOM 1403 CB 204 11.103 LEU 61.362 1.000 21.42 17.486 ANISOU 1403 CB LEU 204 2718 2548 311 2871 -16 - 8

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ATOM
       1404 CG
                     204 9.769
               LEU
                                 18.188
                                         61.079 1.000 33.57
ANISOU 1404 CG LEU
                                         5617
                     204 2820
                                 4319
                                                       -1316 1172
                                                 177
       1405 CD1 LEU
                     204 9.797
MOTA
                                         59.660 1.000 36.19
                                 18.747
ANISOU 1405 CD1 LEU
                     204 4402
                                 3807
                                         5540
                                                1276 -1167 987
                     204 8.581
MOTA
       1406 CD2 LEU
                                 17.234
                                         61.219 1.000 37.76
ANISOU 1406 CD2 LEU
                     204 3058
                                 5328
                                         5960
                                                 -526
                                                       -1896 686
       1407 N
                     205 12.864
ATOM
                GLN
                                 14.836
                                         62.284 1.000 20.33
ANISOU 1407 N
                     205 2518
                GLN
                                 2644
                                         2563
                                                104 - 31 - 129
ATOM
       1408 CA
                GLN
                     205 14.209
                                 14.247
                                         62.335 1.000 18.88
ANISOU 1408 CA
                     205 2522
                GLN
                                 2225
                                         2425
                                                -6 -181
MOTA
       1409 C
                     205 14.512
                GLN
                                 13.504
                                         61.036 1.000 18.19
ANISOU 1409 C
                     205 1986
                GLN
                                 2383
                                         2543
                                                -143
                                                       -188 - 80
MOTA
       1410 O
                     205 13.577
                GLN
                                         60.408 1.000 19.87
                                 13.033
ANISOU 1410 O
                     205 1974
                GLN
                                 3063
                                         2514
                                                -125
                                                      -212 - 237
ATOM
       1411 CB
                     205 14.296
                GLN
                                 13.267
                                         63.493 1.000 24.25
ANISOU 1411 CB
                     205 3948
                GLN
                                 2716
                                         2548
                                                202
                                                       -343296
       1412 CG
ATOM
                     205 14.164
                GLN
                                         64.856 1.000 30.64
                                 13.948
ANISOU 1412 CG
                GLN
                     205 4099
                                 5159
                                         2382
                                                850
                                                       -327 - 89
       1413 CD
ATOM
                GLN
                     205 14.744
                                 13.078
                                         65.948 1.000 28.28
ANISOU 1413 CD GLN
                     205 4473
                                         2640
                                 3633
                                                -161 -1015 -390
       1414 OE1 GLN
ATOM
                     205 14.307
                                 11.921
                                         66.041 1.000 37.69
ANISOU 1414 OE1 GLN
                     205 5733
                                5073
                                         3515
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       1415 NE2 GLN
ATOM
                     205 15.710
                                 13.553
                                         66.711 1.000 40.53
ANISOU 1415 NE2 GLN
                     205 6798
                                 4417
                                         4185
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       1416 N
ATOM
                     206 15.752
                ALA
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                                 13.471
ANISOU 1416 N
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                ALA
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                                         2769
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ATOM
       1417 CA
               ALA
                     206 16.152
                                 12.700
                                         59.405 1.000 18.42
ANISOU 1417 CA
                ALA
                     206 2074
                                 2351
                                         2575
                                                -100
                                                      -15823
ATOM
       1418 C
                     206 17.343
                ALA
                                 11.802
                                         59.738 1.000 17.41
ANISOU 1418 C
                     206 2107
                ALA
                                 2158
                                         2350
                                                -185
                                                      -254 - 17
ATOM
       1419 0
                     206 18.123
                ALA
                                         60.613 1.000 20.67
                                 12.203
ANISOU 1419 O
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                ALA
                                 2410
                                         2973
                                                       -711 - 396
                                                -48
       1420 CB
MOTA
                ALA
                     206 16.637
                                 13.599
                                         58.270 1.000 18.77
ANISOU 1420 CB
                     206 2119
                ALA
                                 2310
                                         2703
                                                156
                                                       -65 147
ATOM
       1421 N
                GLU
                     207 17.492
                                 10.764
                                         58.931 1.000 18.09
ANISOU 1421 N
                GLU
                     207 2092
                                 2101 -
                                         2680
                                                -249 \quad -496 \quad -162
       1422 CA GLU
ATOM
                     207 18.710
                                 9.944
                                         58.966 1.000 19.48
ANISOU 1422 CA
                GLU
                     207 2210
                                 2091
                                         3100
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       1423 C
MOTA
                     207 19.851
                GLU
                                 10.730
                                         58.320 1.000 19.98
ANISOU 1423 C
                GLU
                     207 2018
                                 2233
                                         3342
                                                220
                                                       -560 5 4 4
ATOM 1424 O GLU
                     207 19.732 11.068
                                         57.143 1.000 20.33
ANISOU 1424 O
                GLU
                     207 2000
                                         2970
                                 2753
                                                5 -471 8 9
ATOM
       1425 CB GLU
                     207 18.566
                                 8.623
                                         58.214 1.000 24.03
ANISOU 1425 CB GLU
                     207 3401
                                 1784
                                         3946
                                                      -1226 6 1
                                                316
       1426 CG GLU
ATOM
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                                 7.674
                                         58.295 1.000 24.35
ANISOU 1426 CG GLU
                     207 3223
                                 1907
                                         4121
                                                354 93 4 6 7
MOTA
       1427 CD GLU
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                                 7.791
                                         57.129 1.000 31.69
ANISOU 1427 CD GLU
                     207 2729
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                                         4134
                                                -1218 -175 1 2 2
MOTA
       1428 OE1 GLU
                     207 20.376 7.611
                                         55.943 1.000 26.97
ANISOU 1428 OE1 GLU
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                                 3404
                                         3993
                                                31 -256 309
       1429 OE2 GLU
ATOM
                     207 21.908
                                8.121
                                         57.407 1.000 30.70
ANISOU 1429 OE2 GLU
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                                 3416
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                                                -233 \quad -342 \quad -1168
ATOM
       1430 N
                VAL
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                                 10.936 59.078 1.000 18.53
ANISOU 1430 N
                VAL
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                                         2907
                                                130
                                                       -362320
ATOM
       1431 CA VAL
                     208 22.150 11.547
                                         58.541 1.000 19.53
ANISOU 1431 CA VAL
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                                 2238
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                                                39 -476 630
ATOM
       1432 C
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                VAL
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ANISOU 1432 C
                VAL
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                                         3507
                                                225
                                                       -461 7 9 7
ATOM
                     208 23.460
       1433 O
                VAL
                                 10.663
                                         60.314 1.000 23.82
ANISOU 1433 O
                    208 2262
                VAL
                                         3547 -40
                                 3240
                                                     -858 8 2 5
ATOM
       1434 CB
               VAL
                     208 22.271 13.027 58.905 1.000 19.72
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						60				
ATOM ANISOU ATOM	1448 1449 1445 1451 1451 1451 1455 1455 1455	COCCUMOCOOMMOCOOMMOCOOCOMMOCOOCOMMOCOOCOMMOCOOCO	VVVGGGGGGGGGGGGGGAAAAAAAAAAAPPPPPPPPPTTTTTTTT	22222222222222222222222222222222222222	193.24.30 0 0 1 3 2 0 2 1 2 3 2 3 2 3 2 3 2 3 2 3 2 3 2 3 2 3	-60 - 9 2 6 2 2 9 13 2 13 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1	3293 64.124 2685 65.210 3335 64.388 8288 63.271 3122 63.433 3089 63.400 3560 62.517 3223	1.000 1372 1.000 10.000 1.0000 1.0000	-1177 6 3 2 3 5 . 6 2 -610 9 7 0 3 1 . 4 3 6 9 1 8 5 4 2 8 . 2 8 -551 1 0 1 0 4 1 . 3 6 -18 - 7 9 1 3 6 . 6 8 1265 2 1 7 1 2 8 . 8 2 5 0 4 1 0 3 7 3 4 . 7 2 -539 7 7 6 3 9 . 1 2 -1129 1 2 2 0 4 5 . 3 5 3 7 4 8 2 3 1 4 2 6 . 3 0 -581 1 0 0 2 5 . 0 8 -810 - 3 2 3 2 3 . 8 1 -855 - 6 4 3 2 1 . 4 0 -580 - 1 7 9 2 7 . 6 0 -356 - 7 9 8	
ATOM ANISOU ATOM ANISOU	1458 1458 1459 1459	O O CB CB	THR THR THR THR	213 213 213 213	17.329 2640 20.398 3155	15.137 2269 14.759 3220	62.517 3223 62.308 4113	1.000 -328 1.000 189	21.40 -580 -179 27.60 -356 -798	
ANISOU ATOM ANISOU ATOM ANISOU	1460 1461 1461 1462 1462	OG1 CG2 CG2 N	THR THR THR ASP ASP	213 213 213 214 214	3582 20.735 4422 18.119 2790	4220 16.254 3320 16.177 2236	4356 62.355 3448 64.371 2972	746 1.000 -106 1.000 -82	-410 5 2 0 29.45 -1265 - 204 21.05 -380 - 142	
ATOM ANISOU ATOM ANISOU	1464	CA C	ASP ASP ASP	214 214	17.001 2742 16.994 2373	17.110 2095 18.030 2525	64.462 2993 63.226 2923	-117		

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ATOM
       1465 O
               ASP
                    214 18.018
                                18.430
                                        62.678 1.000 23.02
ANISOU 1465 O
                    214 2461
               ASP
                                2883
                                        3404
                                               -167 -52 -572
                    214 17.205
MOTA
               ASP
       1466 CB
                                18.058
                                        65.637 1.000 23.54
ANISOU 1466 CB
               ASP
                    214 3304
                                2607
                                        3032
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                                                     -748 -668
       1467 CG
ATOM
               ASP
                    214 16.915
                                        67.004 1.000 24.93
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ANISOU 1467 CG ASP
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       1468 OD1 ASP
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ANISOU 1468 OD1 ASP
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       1469 OD2 ASP
ATOM
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ANISOU 1469 OD2 ASP
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MOTA
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ANISOU 1470 N
               LEU
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ATOM
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ANISOU 1471 CA LEU
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MOTA
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ATOM
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ANISOU 1473 O
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              LEU
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ANISOU 1474 CB
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ATOM
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ANISOU 1476 CD1 LEU
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MOTA
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ANISOU 1478 N
               PRO
                    216 2407
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                                        2879
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      1479 CA PRO
ATOM
                    216 14.665
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                                        63.708 1.000 22.42
ANISOU 1479 CA
               PRO
                    216 2869
                                2812
                                                     10 - 228
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                                               272
      1480 C
MOTA
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ANISOU 1480 C
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               PRO
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ANISOU 1481 O
               PRO
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ATOM
      1482 CB
               PRO
                    216 15.693
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ANISOU 1482 CB
               PRO
                    216 3108
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      1483 CG
ATOM
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ANISOU 1483 CG
                    216 2994
               PRO
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      1484 CD PRO
                    216 16.807
ATOM
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ANISOU 1484 CD PRO
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ATOM 1485 N TYR 217 13.154
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ANISOU 1485 N
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      1486 CA
ATOM
               TYR
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ANISOU 1486 CA
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                                               104
      1487 C
ATOM
                    217 13.824 26.516
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                    217 14.570
ATOM
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ANISOU 1488 O
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      1489 CB
ATOM
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ANISOU 1489 CB
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ATOM
      1490 CG
                   217 11.189
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                                27.543 63.125 1.000 31.64
ANISOU 1490 CG TYR
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ATOM
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ANISOU 1491 CD1 TYR
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                                        5314
                                               511
MOTA
      1492 CD2 TYR 217 11.512
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ANISOU 1492 CD2 TYR 217 4721
                                2813
                                        7093
                                               -686 -1682 -749
      1493 CE1 TYR
ATOM
                    217 10.021
                                29.219 61.772 1.000 26.53
ANISOU 1493 CE1 TYR 217 1908
                                2675
                                        5496
                                               -41
                                                     107 6 9
      1494 CE2 TYR
ATOM
                    217 11.113 29.835 63.827 1.000 42.90
ANISOU 1494 CE2 TYR 217 7112
                                2347
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                                             -1415 -1949 - 218
       1495 CZ TYR
ATOM
                    217 10.373 30.168 62.712 1.000 34.93
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MOTA
       1526 O
                     221 13.763
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               ALA
                                        56.415 1.000 26.47
ANISOU 1526 O
               ALA
                     221 4127
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                                        3289
                                               -1307894 - 904
                    221 16.939 28.316
MOTA
       1527 CB
               ALA
                                        56.104 1.000 19.36
ANISOU 1527 CB
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MOTA
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ANISOU 1528 N
                    222 2089
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                                                     -323 - 154
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                    222 13.556 26.276
ATOM
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ANISOU 1529 CA
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               VAL
                    222 1620
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ATOM
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               VAL
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ANISOU 1530 C
                    222 1616
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ATOM
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                                        53.716 1.000 17.84
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               VAL
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                                        3390
                                               -108 -194 4 8
ATOM
       1532 CB
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ANISOU 1532 CB VAL
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       1533 CG1 VAL
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ANISOU 1533 CG1 VAL
                    222 2252
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                                        2977
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                                                     -645 - 182
       1534 CG2 VAL
                    222 11.730 25.411.
ATOM
                                        52.490 1.000 22.44
ANISOU 1534 CG2 VAL
                    222 2923
                                2537
                                        3067
                                               -497
                                                     -898 4 4
       1535 N
ATOM
                    223 13.789 23.892
               LEU
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ANISOU 1535 N
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                    223 1792
                                1694
                                        2706
                                               -239 -93 -532
       1536 CA LEU
MOTA
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                                        54.579 1.000 15.91
ANISOU 1536 CA
               LEU
                    223 1679
                                1864
                                        2503
                                                     -297 - 333
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       1537 C
MOTA
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                    223 1337
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                                               -141 -322 - 458
ATOM
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                    223 12.969 21.888
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ANISOU 1538 O
               LEU
                    223 1317
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ATOM
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ANISOU 1539 CB
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MOTA
       1540 CG
              LEU
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ANISOU 1540 CG LEU
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ATOM
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ANISOU 1541 CD1 LEU
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                                               69 135 3 1 6
       1542 CD2 LEU
ATOM
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ANISOU 1542 CD2 LEU
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                                3296
                                        7459
                                               525
                                                     1116 2 3 3 3
ATOM
       1543 N
                    224 15.115
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ATOM
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ANISOU 1545 C
                    224 1464
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ATOM 1546 O VAL 224 16.442 18.861 51.981 1.000 15.38
ANISOU 1546 O
                    224 1464
               VAL
                                1558
                                        2822
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MOTA
       1547 CB VAL 224 15.832 21.209
                                        50.222 1.000 14.25
ANISOU 1547 CB VAL
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ANISOU 1548 CG1 VAL
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                                               -159 - 408 - 421
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       1549 CG2 VAL
ATOM
                    224 15.575
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ANISOU 1549 CG2 VAL
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                                        2863
                                               6 -509 8 7
       1550 N
               PHE
ATOM
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                                        51.299 1.000 13.49
ANISOU 1550 N
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                     225 1494
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ANISOU 1551 CA PHE
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                                        2431
       1552 C
ATOM
               PHE
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                                        49.675 1.000 14.27
ANISOU 1552 C
                     225 1536
               PHE
                                1533
                                        2352
                                                     -260 - 194
                                               100
ATOM
       1553 O
                     225 13.858 16.876
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ANISOU 1553 O
                     225 1604
               PHE
                                               296
                                                     -311 - 88
                                2000
                                        2569
       1554 CB PHE
ATOM
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ANISOU 1554 CB PHE
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                                1563
                                        2740
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                                                     -46 2 4
       1555 CG PHE
ATOM
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                                        53.257 1.000 17.95
ANISOU 1555 CG PHE
                     225 1888
                                        2666 -650 -302 2 0 3
                                2267
       1556 CD1 PHE
ATOM
                     225 14.409 15.809
                                        54.157 1.000 27.39
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ANISOU 1556 CD1 PHE
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       1557 CD2 PHE
ATOM
                     225 12.125
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ANISOU 1557 CD2 PHE
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                                                  -166 399 -527
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ANISOU 1559 CE2 PHE
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MOTA
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                     225 3705
ANISOU 1560 CZ
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ANISOU 1561 N
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                CYS
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       1562 CA
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ATOM
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                CYS
ANISOU 1562 CA
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ATOM
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ANISOU 1563 C
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ATOM
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ANISOU 1564 O
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ATOM
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ANISOU 1565 CB
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       1566 SG
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ATOM
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ANISOU 1566 SG
                CYS
                     226 1744
                                  1740
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ATOM
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ANISOU 1567 N
                GLY
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                                                        -293 - 290
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       1568 CA
                GLY
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ATOM
                                 12.496
                                          46.899 1.000 12.58
ANISOU 1568 CA
                \mathsf{GLY}
                     227 1279
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                                                  -83
                                          1872
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                     227 13.903
ATOM
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                GLY
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                                  11.541
ANISOU 1569 C
                GLY
                     227 1518
                                  1279
                                          1965
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       1570 O
ATOM
                GLY
                     227 14.917
                                          45.152 1.000 13.58
                                  11.732
ANISOU 1570 O
                GLY
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                                          2008
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ATOM
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ANISOU 1571 N
                     228 1490
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                                          2151
                                                  59 - 204
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ATOM
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                ALA
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ANISOU 1572 CA
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       1573 C
ATOM
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ANISOU 1573 C
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ATOM
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ANISOU 1574 O
                     228 1717
                ALA
                                  1462
                                          2004
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       1575 CB
ATOM
                ALA
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ANISOU 1575 CB
                ALA
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                                          2356
                                                  -219 358 -243
       1576 N
ATOM
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                ILE
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ANISOU 1576 N
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                                          2441
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       1577 CA
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MOTA
                ILE
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ANISOU 1577 CA
                ILE
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                                  1243
                                          2344
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                                                        -306 1 7 3
ATOM
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ANISOU 1578 C
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                ILE
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                                           2311
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ATOM
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                ILE
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ANISOU 1579 O
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                     229 1587
                                  1596
                                           2293
                                                  -37
                                                        -167183
ATOM
       1580 CB
                ILE
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                                  11.888
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ANISOU 1580 CB
                      229 1470
                ILE
                                  1631
                                           2015
                                                  171
                                                        -354 - 42
       1581 CG1 ILE
ATOM
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ANISOU 1581 CG1 ILE
                     229 1218
                                  1936
                                           2817
                                                  85 31 1 1 8
       1582 CG2 ILE
MOTA
                     229 12.040
                                 12.674
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ANISOU 1582 CG2 ILE
                     229 1670
                                  1425
                                                  76 - 364 174
                                           2298
       1583 CD1 ILE
ATOM
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                                 9.924
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ANISOU 1583 CD1 ILE
                      229 2129
                                  1814
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                                                  -208 -385 -488
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ATOM
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                ALA
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ANISOU 1584 N
                      230 1252
                 ALA
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                                           2454
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ATOM
       1585 CA
                ALA
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ANISOU 1585 CA
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ATOM
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                 ALA
                                           41.976 1.000 12.89
ANISOU 1586 C
                 ALA
                      230 1491
                                  1327
                                           2079
                                                  128
                                                        30 - 20
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ANISOU 1587 O AI ATOM 1588 CB AI ANISOU 1588 CB AI ANISOU 1589 N TH ANISOU 1590 CA TH ANISOU 1591 C TH ANISOU 1592 O TH ANISOU 1593 CB TH ANISOU 1593 CB TH ANISOU 1594 OG1 TH ANISOU 1594 OG1 TH ANISOU 1595 CG2 TH ANISOU 1596 N LE ANISOU 1596 N LE ANISOU 1597 CA LE ANISOU 1597 CA LE ANISOU 1598 C LE ANISOU 1598 C LE ANISOU 1599 O LE ANISOU 1599 O LE ANISOU 1599 O LE ANISOU 1599 O LE ANISOU 1600 CB LE ANISOU 1600 CB LE ANISOU 1601 CG LE ANISOU 1601 CG LE ANISOU 1602 CD1 LE ANISOU 1602 CD1 LE ANISOU 1603 CD2 LE ANISOU 1603 CD2 LE ANISOU 1604 N VA ANISOU 1604 N VA ANISOU 1605 CA VA ANISOU 1606 C VA ANISOU 1607 O VA ANISOU 1608 CB VA ANISOU 1609 CG1	HR 231 18.698 7.621 HR 231 1449 1419 EU 232 16.665 9.049 EU 232 16.446 8.396 EU 232 16.975 9.248 EU 232 16.975 9.248 EU 232 16.975 9.248 EU 232 1968 1557 EU 232 17.749 8.808 EU 232 2024 1949 EU 232 14.940 8.135 EU 232 1692 1630 EU 232 1692 1630 EU 232 15.118 5.920 EU 232 15.118 5.920 EU 232 15.118 5.920 EU 232 15.118 5.920 EU 232 16.539 10.514 EU 232 16.539 10.514 AL 233 16.539 10.514 AL 233 16.893 11.317 AL 233 16.893 11.317 AL 233 16.893 11.317 AL 233 16.893 11.510 AL 233 16.893 12.626 AL 233 16.940 11.587 AL 233 16.098 12.626 AL 233 16.098 12.626 AL 233 16.529 13.650	41.146 1.000 13.65 2418 103 4 4 6 43.345 1.000 13.65 2215 -186 -21 -229 42.805 1.000 13.31 2214 58 -261 - 1 42.659 1.000 13.32 2093 78 -302 3 2 41.251 1.000 13.27 2111 205 -211 3 40.620 1.000 15.51 2667 245 58 -170 43.688 1.000 13.03 2151 46 -166 1 2 44.995 1.000 14.70 2230 -99 32 - 14 43.697 1.000 13.69 2335 113 -211 1 9 7 40.796 1.000 13.43 271 75 -404 -2 7 39.527 1.000 14.11 2326 80 -468 4 9 38.381 1.000 15.53 2376 209 -3 9 0 37.504 1.000 15.53 2376 209 -3 9 0 37.504 1.000 17.16 2546 107 -116 -519 39.368 1.000 15.89 2329 120 -470 -3 0 3 38.202 1.000 23.19 3228 743 -1110 -851 38.155 1.000 15.89 2329 120 -470 -3 0 3 38.202 1.000 23.19 3228 743 -1110 -851 38.126 1.000 19.46 3126 -470 -523 -66 38.299 1.000 13.73 2025 -7 -263 1 9 3 37.117 1.000 13.84 1926 141 -73 1 0 7 37.025 1.000 14.08 1958 72 -46 1 1 3 35.910 1.000 16.65 2079 38 109 4 0 1 37.062 1.000 15.70 2698 34 156 -28 35.647 1.000 15.43
ATOM 1604 N VA ANISOU 1604 N VA ATOM 1605 CA VA ANISOU 1605 CA VA	EU 232 2006 2262 AL 233 16.539 10.514 AL 233 1736 1454 AL 233 16.893 11.317 AL 233 1674 1658	3126 -470 -523 - 66 38.299 1.000 13.73 2025 -7 -263 193 37.117 1.000 13.84 1926 141 -73 107
ANISOU 1606 C VA ATOM 1607 O VA ANISOU 1607 O VA ATOM 1608 CB VA ANISOU 1608 CB VA	AL 233 1716 1674 AL 233 18.940 11.587 AL 233 1923 2325 AL 233 16.098 12.626 AL 233 1680 1696	1958 72 -46 1 1 3 35.910 1.000 16.65 2079 38 109 4 0 1 37.062 1.000 14.69
ANISOU 1609 CG1 VA ATOM 1610 CG2 VA ANISOU 1610 CG2 VA ATOM 1611 N TH	AL 233 1615 1654 AL 233 16.117 13.206 AL 233 1740 2041	38.113 1.000 15.70 2698 34 156 - 28 35.647 1.000 16.43 2459 251 117 596 38.175 1.000 14.23
ATOM 1612 CA TH ANISOU 1612 CA TH ATOM 1613 C TH ANISOU 1613 C TH ATOM 1614 O TH	HR 234 20.524 11.908 HR 234 1664 1868 HR 234 21.346 10.621 HR 234 1717 1865 HR 234 22.558 10.644	2083 146 -110 2 3 5 38.148 1.000 16.14 2602 63 -171 - 4 9 38.006 1.000 17.09 2912 146 211 - 5 1 38.139 1.000 17.25
ATOM 1615 CB TH	HR 234 1667 1502 HR 234 20.849 11.819 HR 234 1659 1708	2828 108 200 229 39.373 1.000 15.29 2642 -46 -149 163 40.522 1.000 15.45 2502 -80 59 4 4 39.597 1.000 16.61

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						- 66 -		
ANISOU	1617	CG2	THR	234	1564	1672	3077	3 -34 - 42
ATOM	1618		GLY		20.712	9.441		1.000 15.80
ANISOU	1618		GLY		1905	1914		
ATOM	1619		GLY	235			2564	193 29 - 219
						8.209	37.792	
ANISOU	1619		GLY		2049	1861	2586	133 223 - 488
ATOM	1620	-	GLY		22.225	7.931	39.083	1.000 18.06
ANISOU	1620	C	GLY	235	2046	2049	2768	419 499 303
MOTA	1621	0	GLY		23.285	7.289	39.010	1.000 21.26
ANISOU	1621	0	GLY		2167	2606	3303	679 343 - 74
ATOM	1622		GLY		21.602	8.149		
ANISOU	1622		GLY		1663		40.237	1.000 15.17
ATOM	1623					1901	2582	36 291 3 0 5
			GLY		22.080	7.673	41.520	1.000 17.27
ANISOU	1623		GLY		2135	1671	2754	225 28 2 2 9
ATOM	1624	_	GLY		23.033	8.639	42.194	1.000 16.88
ANISOU	1624		GLY	236	1880	1890	2644	204 100 222
ATOM	1625	0	GLY	236	23.692	8.272	43.193	1.000 19.42
ANISOU	1625	0	GLY	236	2165	2399	2814	314 -90 419
ATOM	1626	N	GLN		23.134	9.890	41.746	
ANISOU	1626	N	GLN		1647	1851	2957	
ATOM	1627		GLN		24.074			213 -213 1 6 7
ANISOU	1627		GLN			10.849	42.298	1.000 16.75
ATOM					1608	2004	2752	72 177 9 8
		C	GLN		23.481	11.604	43.483	1.000 15.64
ANISOU	1628	C	GLN		1404	2136	2402	231 -146 2 0 0
ATOM	1629	0	GLN		24.183	12.382	44.164	1.000 18.17
ANISOU	1629	0	GLN	237	1581	2508	2817	-227 -6 -46
ATOM	1630	CB	GLN	237	24.456	11.855	41.217	1.000 17.17
ANISOU	1630	CB	GLN	237	1912	2080	2532	71 141 - 7
ATOM	1631	CG	GLN		25.304	11.221	40.115	1.000 17.64
ANISOU	1631		GLN		1850	2410	2441	
ATOM	1632		GLN	237	25.721			
ANISOU	1632		GLN	237		12.302	39.137	1.000 19.72
ATOM	1633				1680	2833	2979	104 317 3 0 7
			GLN	237		13.110	39.436	1.000 24.27
ANISOU	1633				1841	3145	4234	-213 -187 8 0 9
MOTA	1634			237	24.986	12.399	38.027	1.000 18.53
ANISOU	1634		GLN	237	2007	2298	2735	432 374 202
$\mathtt{ATOM}$	1635	N	VAL	238	22.221	11.359	43.807	1.000 14.75
ANISOU	1635	N	VAL	238	1563	1804	2237	-32 -54 4 3
ATOM	1636	CA	VAL	238	21.533	12.075	44.862	1.000 14.41
ANISOU	1636	CA	VAL		1535	1553	2388	0 -44 3 2
ATOM	1637	C	VAL	238	20.861	11.060	45.781	1.000 13.56
ANISOU	1637	_	VAL	238	1414	1392		
ATOM		Ö	VAL	238	20.136		2346	82 55 - 149
ANISOU	1638	0	VAL			10.174	45.302	1.000 15.87
ATOM	1639			238	1655	1639	2737	<b>-218 -285 -22</b>
			VAL	238	20.467	13.061	44.309	1.000 14.73
ANISOU	1639		VAL	238	1817	1626	2152	35 -437 - 95
ATOM	1640			238	19.805	13.764	45.489	1.000 15.70
ANISOU				238	1965	1490	2510	174 -524 - 423
ATOM	1641			238	21.064	13.994	43.280	1.000 16.82
ANISOU	1641	CG2	VAL	238	1862	1718	2812	-60 -378 2 2 2
ATOM	1642		LYS		21.119	11.153	47.071	1.000 14.47
ANISOU	1642		LYS		1704	1474	2318	
ATOM	1643		LYS		20.470			14 -40 1 2
	1643					10.360		1.000 14.43
ATOM			LYS		1460	1617	2406	106 -168 1 7 9
	1644		LYS	239		10.852		1.000 14.82
ANISOU	1644		LYS		1533	1456	2642	102 -53 232
ATOM	1645		LYS	239	18.839	12.067	48.457	1.000 14.74
ANISOU			LYS	239	1841	1442	2318	158 -275 1 9 0
ATOM	1646	CB	LYS	239	21.320	10.435	49.385	
ANISOU	1646	CB	LYS		1995	1712	2527	243 -543 2 5 2
ATOM	1647		LYS		20.767	9.549	50.498	
ANISOU			LYS		1954	1759	2614	
	,			~ 5 5	<b>-</b>	1177	7 0 T #	-58 -781 2 4 4

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- 67 -MOTA 239 21.738 9.511 1648 CD LYS 51.683 1.000 19.76 ANISOU 1648 CD LYS 239 2954 1820 -123 -1234 363 2732 239 21.107 8.835 ATOM 1649 CE LYS 52.896 1.000 22.58 ANISOU 1649 CE LYS 239 3331 2164 3086 -652 -1502 863 239 21.904 8.883 ATOM 1650 NZ LYS 54.145 1.000 23.13 ANISOU 1650 NZ LYS 239 2817 3360 2612 -471 -943 2 8 7 ATOM 1651 N ALA 240 18.140 9.892 48.659 1.000 14.35 ANISOU 1651 N ALA 240 1429 1607 2418 -156 -334 - 61 1652 CA ATOM ALA 240 16.791 49.145 1.000 13.98 10.192 ANISOU 1652 CA ALA240 1468 1635 2210 -151 -335 - 10 1653 C ATOM ALA 240 16.728 9.776 50.605 1.000 13.44 ANISOU 1653 C 240 1439 ALA 1388 2279 77 -450 ATOM 1654 0 ALA 240 16.514 8.592 50.913 1.000 16.32 ANISOU 1654 O ALA 240 1932 1567 2699 -215 -673314ATOM 1655 CB ALA 240 15.712 9.565 48.268 1.000 15.21 ANISOU 1655 CB ALA 240 1510 2306 1962 -104 -387 -307ATOM 1656 N PRO 241 16.907 51.546 1.000 14.23 10.701 ANISOU 1656 N PRO 241 1634 1551 2221 -87 -292 7 1 1657 CA ATOM 10.251 PRO 241 17.035 52.940 1.000 14.68 ANISOU 1657 CA PRO 2180 241 1718 1681  $-350 \quad -174 \quad -30$ 1658 C ATOM PRO 241 15.693 53.579 1.000 13.89 9.961 ANISOU 1658 C PRO 241 1659 1581 2039 -107 - 207 - 74ATOM 1659 0 241 14.629 PRO 10.527 53.261 1.000 17.06 ANISOU 1659 0 PRO 241 1698 1946 17 -254 146 2838 1660 CB ATOM PRO 241 17.689 53.619 1.000 16.63 11.462 ANISOU 1660 CB 241 2162 PRO 1657 **-460 -487** 5 5 2501 1661 CG ATOM PRO 241 17.138 12.651 52.826 1.000 16.56 ANISOU 1661 CG PRO 241 - 2433 1601 2258 -367 -274311662 CD ATOM 241 17.164 12.140 PRO 51.409 1.000 14.92 ANISOU 1662 CD 241 1841 PRO 1490 2339 -215 -186 - 66 1663 N ATOM ARG 242 15.740 54.544 1.000 15.74 9.049 ANISOU 1663 N ARG 242 1914 1853 2212 -308 2 0 4 -381 1664 CA ATOM ARG 242 14.574 8.772 55.376 1.000 15.50 ANISOU 1664 CA ARG 242 1955 1863 2073 -236 -291 1 8 0 ATOM 1665 C 242 14.406 ARG 9.841 56.437 1.000 16.60 ANISOU 1665 C 242 1889 ARG 2407 -1202011 -411 - 511666 0 ATOM ARG 242 15.372 10.416 56.994 1.000 18.31 ANISOU 1666 O ARG 242 2041 -216 -559 -180 2186 2732 ATOM 1667 CB 242 14.728 7.419 ARG 56.085 1.000 18.38 ANISOU 1667 CB ARG 242 2920 1810 2253 -486 -391 2 6 9 ATOM 1668 CG ARG 242 14.564 6.273 55.094 1.000 18.42 ANISOU 1668 CG ARG 242 2372 1873 2755 -88 162 - 155 1669 CD ARG ATOM 242 14.854 4.935 55.796 1.000 23.07 ANISOU 1669 CD ARG 242 3380 2022 3366 470 -483 - 217ATOM 1670 NE ARG 242 16.334 4.954 55.991 1.000 26.69 ANISOU 1670 NE ARG 242 3498 2727 3916 444 -829 4 7 1671 CZ ARG ATOM 242 16.941 3.921 -56.584 1.000 27.19 ANISOU 1671 CZ ARG 242 3166 2879 4284 -297 -1143 802 1672 NH1 ARG ATOM 242 16.157 2.913 56.989 1.000 33.14 ANISOU 1672 NH1 ARG 242 3810 3235 -316 528 726 5546 1673 NH2 ARG ATOM 242 18.241 3.889 56.779 1.000 31.13 ANISOU 1673 NH2 ARG 242 3043 2925 5859 227 -769 4 8 4 1674 N MOTA 243 13.188 10.057 HIS 56.872 1.000 17.55 ANISOU 1674 N HIS 243 1979 -165 -173 - 74 2233 2457 1675 CA HIS ATOM 243 12.913 11.050 57.914 1.000 17.84 ANISOU 1675 CA HIS 2139 243 2186 2452 -260 -123 - 75ATOM 1676 C 243 11.644 10.627 HIS 58.643 1.000 17.52 ANISOU 1676 C HIS 243 2102 2470 -248 -164 - 325 2084 243 10.870 9.803 1677 0 ATOM HIS 58.132 1.000 20.23 ANISOU 1677 O HIS 243 2226 2593 2868 -551 -323 -392 ATOM 1678 CB HIS 243 12.865 12.456 57.324 1.000 19.74

	- 68 -	
ANISOU 1678 CB HIS	243 2770 2248 2482	
ATOM 1679 CG HIS	243 11.922 12.630 56.1	
ANISOU 1679 CG HIS	243 3449 2513 2624	
ATOM 1680 ND1 HIS	243 12.209 12.299 54.8	
ANISOU 1680 ND1 HIS ATOM 1681 CD2 HIS	243 4780 2575 2473	-609 -403 5 3
ANISOU 1681 CD2 HIS		72 1.000 29.11
ATOM 1682 CE1 HIS		_
ANISOU 1682 CE1 HIS	243 11.182 12.573 54.1 243 5835 3672 3001	
ATOM 1683 NE2 HIS		-1102 -1367 689 75 1.000 36.95
ANISOU 1683 NE2 HIS	243 5719 4201 4119	
ATOM 1684 N HIS		31: 1.000 18.87
ANISOU 1684 N HIS	244 2523 2477 2171	
ATOM 1685 CA HIS		49 1.000 20.83
ANISOU 1685 CA HIS	244 2802 2485 2628	
ATOM 1686 C HIS		51 1.000 20.33
ANISOU 1686 C HIS	244 1803 2969 2953	-31 -78 -273
ATOM 1687 O HIS	• • •	10 1.000 21.71
ANISOU 1687 O HIS	244 2057 3418 2774	
ATOM 1688 CB HIS ANISOU 1688 CB HIS	<b>*</b> • • • • • • •	68 1.000 24.38
ANISOU 1688 CB HIS ATOM 1689 CG HIS	244 4066 2644 2553	
ANISOU 1689 CG HIS	244 11.859 9.725 62.4 244 4158 3498 3113	
ATOM 1690 ND1 HIS	244 4158 3498 3113 244 13.132 9.205 62.2	
ANISOU 1690 ND1 HIS	244 4012 4471 3808	
ATOM 1691 CD2 HIS	244 11.928 10.391 63.6	
ANISOU 1691 CD2 HIS	244 2937 4137 2505	
ATOM 1692 CE1 HIS	244 13.887 9.531 63.3	
ANISOU 1692 CE1 HIS	244 4157 4277 3613	1224 -749 - 518
ATOM 1693 NE2 HIS	244 13.146 10.263 64.1	
ANISOU 1693 NE2 HIS	244 3165 3517 2633	
ATOM 1694 N VAL ANISOU 1694 N VAL	245 8.890 11.687 62.3	
ANISOU 1694 N VAL ATOM 1695 CA VAL	245 2627 3119 3322	
ANISOU 1695 CA VAL	245 8.473 12.691 63.3 245 2785 3770 2888	
ATOM 1696 C VAL	245 2785 3770 2888 245 8.624 12.079 64.7	
ANISOU 1696 C VAL	245 3220 3558 3112	
ATOM 1697 O VAL	245 8.023 11.025 64.9	
ANISOU 1697 O VAL	245 3120 3085 4428	
ATOM 1698 CB VAL	245 7.020 13.114 63.0	
ANISOU 1698 CB VAL	245 2621 3489 3777	94 -103 -569
ATOM 1699 CG1 VAL	245 6.586 14.114 64.1	61 1.000 28.06
ANISOU 1699 CG1 VAL	245 2717 3330 4614	
ATOM 1700 CG2 VAL	245 6.927 13.705 61.6	
ANISOU 1700 CG2 VAL ATOM 1701 N ALA	245 3564 3809 4220	
		03 1.000 28.08
ANISOU 1701 N ALA ATOM 1702 CA ALA	246 4338 3787 2543 246 9.567 12.316 67.0	
ANISOU 1702 CA ALA	246 9.567 12.316 67.0 246 4363 3360 2707	
ATOM 1703 C ALA		33 1.000 32.68
ANISOU 1703 C ALA		98 880 1 9 7
ATOM 1704 O ALA		63 1.000 29.54
ANISOU 1704 O ALA	246 3522 4283 3417	
ATOM 1705 CB ALA		42 1.000 30.33
ANISOU 1705 CB ALA	246 4564 3949 3011	
ATOM 1706 N ALA		49 1.000 34.09
ANISOU 1706 N ALA	<b>.</b>	-1190 466 3 9 3
ATOM 1707 CA ALA		59 1.000 34.23
ANISOU 1707 CA ALA		-1215 315 5 1 5
ATOM 1708 C ALA ANISOU 1708 C ALA		081 1.000 33.31
ANISOU 1708 C ALA	247 5419 4684 2555	5 249 -506 1 1 4 7

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- 69 -ATOM 1709 O ALA247 8.733 12.708 71.523 1.000 38.23 ANISOU 1709 O 247 5787 ALA 4478 -378 -1519 1230 4259 ATOM 1710 CB 247 6.383 ALA 10.881 70.314 1.000 47.11 ANISOU 1710 CB 247 8374 ALA -2800 1464 686 6726 2801 ATOM 1711 N 248 6.817 PRO 13.851 71.577 1.000 42.28 ANISOU 1711 N 248 5771 PRO 5458 4836 -300 933 - 97 ATOM 1712 CA PRO 248 7.256 72.773 1.000 44.85 14.581 ANISOU 1712 CA 248 7568 PRO 5478 3996 -645 1413 2 1 4 1713 C ATOM PRO 248 7.161 13.618 73.948 1.000 49.25 248 7978 ANISOU 1713 C PRO 5660 5075 -1446 552 985 ATOM 1714 0 PRO 248 6.251 12.794 74.014 1.000 45.48 ANISOU 1714 O PRO 248 7651 5391 4237 -1127 2573 - 796 1715 CB ATOM 248 6.196 PRO 15.674 72.897 1.000 49.75 ANISOU 1715 CB PRO 248 8563 4816 5523 -513 1238 -138 1716 CG ATOM PRO 248 4.973 15.053 72.299 1.000 50.89 ANISOU 1716 CG 248 7228 PRO 5564 6545 -108 2210 -1064 1717 CD ATOM 14.272 PRO 248 5.489 71.114 1.000 44.69 ANISOU 1717 CD 248 6395 PRO 4579 6006 937 953 - 577 1718 N ATOM 249 8.109 ARG 74.883 1.000 48.76 13.683 ANISOU 1718 N 249 9141 ARG 6341 3045 -1317 1069 - 477 1719 CA 249 7.865 ATOM ARG 76.024 1.000 55.51 12.783 ANISOU 1719 CA 249 10023 ARG 6914 -1098 895 4156 ATOM 1720 C ARG 249 6.844 13.466 76.916 1.000 46.09 ANISOU 1720 C 249 5561 ARG 8382 3568 -2484 - 7 1237ATOM 1721 0 ARG 249 6.244 12.915 77.831 1.000 56.25 ANISOU 1721 O ARG 249 7572 6368 7433 -377 1799 3995 1722 CB ATOM ARG 249 9.177 12.459 76.721 1.000 55.24 ANISOU 1722 CB ARG 249~8950 7715 4326 2864 1270 705 ATOM 1723 CG ARG 249 9.915 11.278 76.110 1.000 71.04 ANISOU 1723 CG 249 12881 ARG 7330 3707 6 2 2 1135 6779 MOTA 1724 CD 249 10.403 ARG 10.303 77.165 1.000 72.89 ANISOU 1724 CD ARG 249 11721 7991 7984 2171 2723 4 0 9 ATOM 1725 NE ARG 249 11.124 9.162 76.580 1.000 70.73 ANISOU 1725 NE 249 8627 ARG 9977 8271 2650 - 266 2362 1726 CZ ATOM 249 12.039 ARG 77.282 1.000 72.71 8.493 ANISOU 1726 CZ ARG 249 10269 9417. 7942 2304 2153 1 3 3 1727 NH1 ARG MOTA 249 12.297 78.521 1.000 89.50 8.893 ANISOU 1727 NH1 ARG 249 22286 6161 5559 2015 1622 3874 1728 NH2 ARG ATOM 249 12.682 7.462 76.761 1.000 67.68 ANISOU 1728 NH2 ARG 249 5358 10062 10295 1004 3886 2 2 1 ATOM 1729 N ALA 254 1.981 18.918 75.430 1.000 85.24 ANISOU 1729 N ALA 254 15501 7922 -4581 -1437 2347 8964 ATOM 1730 CA ALA 254 2.287 76.257 1.000 76.08 20.081 ANISOU 1730 CA 254 12510 ALA 8110 -3993 1617 1592 8286 ATOM 1731 C 254 2.943 21.216 ALA 75.489 1.000 60.91 ANISOU 1731 C 254 8383 ALA 5719 9040 -506 2886 1312 1732 0 MOTA 21.309 ALA 254 4.174 75.487 1.000 72.37 ANISOU 1732 O ALA 254 8056 8109 11332 1602 4553 3381 1733 CB ATOM 254 3.264 ALA 19.667 77.351 1.000 60.48 ANISOU 1733 CB 254 12589 ALA 7262 3131 -866 4570 -1112 MOTA 1734 N 255 2.200 GLY 74.846 1.000 54.40 22.108 ANISOU 1734 N 255 8029 GLY 5451 7190 594 2922 - 9401735 CA MOTA GLY 255 2.880 23.171 74.098 1.000 40.05 ANISOU 1735 CA GLY 255 5181 4570 5465 1424 836 -921 1736 C MOTA GLY 255 3.640 72.921 1.000 38.82 22.565 ANISOU 1736 C GLY 255 4227 4772 5749 557 702 -1561 ATOM 1737 0 GLY 255 4.580 72.398 1.000 39.96 23.163 ANISOU 1737 O GLY 255 2978 6491 5715 -128 -136 -2226 ATOM 1738 N SER 256 3.164 21.387 72:509 1.000 37.29 ANISOU 1738 N SER 256 5047 4594 4527 389 11 -853 MOTA 1739 CA SER 256 3.738 71.429 1.000 35.71 20.606

ANISOU 1739 CA SER 256 4737 4533 4299 560 -501 - 9191740 C 256 2.983 ATOM SER 20.742 70.118 1.000 34.93 ANISOU 1740 C 256 4584 SER 4669 4019 -98 -85 9 1 1741 0 ATOM SER 256 3.251 69.162 1.000 33.92 20.000 ANISOU 1741 O SER 256 3575 6107 3207 503 304 377 256 3.845 ATOM 1742 CB SER 71.853 1.000 30.17 19.136 256 3125 ANISOU 1742 CB SER 4830 3509 624 212 - 492ATOM 256 2.688 1743 OG SER 18.752 72.601 1.000 61.15 256 2987 ANISOU 1743 OG SER 8497 11750 451 1943 2630 257 2.065 21.700 ATOM 1744 N SER 70.030 1.000 35.54 ANISOU 1744 N 257 4037 5989 SER 3479 347 242 - 861745 CA 257 1.379 MOTA SER 21.993 68.767 1.000 30.95 ANISOU 1745 CA 257 2824 SER 5827 3109 170 672 - 509 1746 C ATOM 257 2.378 SER 22.538 67.760 1.000 30.63 ANISOU 1746 C 257 3181 SER 5524 -476 765 -1297 2934 1747 0 ATOM SER 257 3.359 68.199 1.000 34.70 23.159 ANISOU 1747 O 257 3500 SER 6070 3616 -829 603 -1516 1748 CB 257 0.331 ATOM SER 23.088 69.036 1.000 38.70 ANISOU 1748 CB 6518 SER 257 3085 5103 1381 4 3 5 796 1749 OG ATOM 257 0.801 SER 24.361 68.601 1.000 65.12 ANISOU 1749 OG SER 257 8002 5175 11565 -999 -3375 383 1750 N ATOM ARG 258 2.119 22.384 66.471 1.000 30.51 ANISOU 1750 N ARG 258 3668 5068 2855 -332 677 - 9951751 CA ARG 258 2.997 ATOM 22.819 65.396 1.000 28.15 ANISOU 1751 CA ARG 258 3100 4620 2976 -106 358 -544 1752 C 258 2.198 ATOM 22.913 ARG 64.096 1.000 25.64 ANISOU 1752 C ARG 258, 3488 3381 2872 -676 273 -904 1753 0 ATOM ARG 22.294 63.981 1.000 24.93 258 1.132 258 3162 ANISOU 1753 O ARG 3240 -441 478 -5603070 ATOM 1754 CB ARG 258 4.175 65.154 1.000 27.21 21.873 ANISOU 1754 CB ARG 258 3158 3141 4041 -446 313 -1352 1755 CG MOTA 258 3.861 20.508 ARG 64.570 1.000 30.90 ANISOU 1755 CG 258 4782 ARG 3429 3531 **-737 -738 -389** ATOM 1756 CD ARG 258 5.039 19.537 64.769 1.000 36.65 ANISOU 1756 CD ARG 258 5937 3466 4523 106 477 3 0 6 1757 NE ATOM ARG 258 4.597 64.411 1.000 32.42 18.176 ANISOU 1757 NE 258. 3372 ARG 3858 -2745285089 -85 1758 CZ 258 4.633 ATOM 63.143 1.000 37.32 ARG 17.777 ANISOU 1758 CZ ARG 258 5670 2958 5553 155 680 4 3 ATOM 1759 NH1 ARG 258 5.075 18.622 62.217 1.000 29.98 ANISOU 1759 NH1 ARG 258 3077 3435 4881 -150 -211 -103 1760 NH2 ARG 258 4.210 ATOM 16.566 62.824 1.000 38.66 ANISOU 1760 NH2 ARG 258 5812 -190 -1632 865 3151 5724 ATOM 1761 N 259 2.806 23.572 THR 63.120 1.000 23.62 ANISOU 1761 N THR 259 2625 3578 2771 -519 315 -1037 ATOM 1762 CA THR 259 2.337 61.730 1.000 21.97 23.482 ANISOU 1762 CA THR 259 2614 2934 2800 -36 247 - 1041ATOM 1763 C 259 3.528 THR 23.197 60.808 1.000 19.76 ANISOU 1763 C THR 259 2257 2663 2587 -38 21 - 699ATOM 1764 0 THR 259 4.698 61.159 1.000 21.13 23.411 ANISOU 1764 O THR 259 2464 3096 2468 -495 -10 -2861765 CB THR ATOM 259 1.682 24.793 61.278 1.000 24.04 ANISOU 1765 CB THR 259 2125 3084 3927 70 -157 -1229 1766 OG1 THR ATOM 259 2.697 61.041 1.000 23.14 25.790 ANISOU 1766 OG1 THR 259 2297 2848 3648 -142 - 829196 1767 CG2 THR ATOM 259 0.760 62.331 1.000 25.17 25.408 ANISOU 1767 CG2 THR 259 2941 3229 3393 726 264 - 136ATOM 1768 N 22.706 59.600 1.000 20.41 SER 260 3.234 ANISOU 1768 N SER 260 2386 2762 2609 -61 74 - 806 ATOM 1769 CA SER 22.515 260 4.225 58.551 1.000 19.33 ANISOU 1769 CA 260 2488 SER 2459 2399 192 8 - 344

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MOTA 1770 C SER 22.871 57.210 1.000 18.78 260 3.587 ANISOU 1770 C SER 260 1996 2544 2595 -379 -264 - 311ATOM 260 2.375 1771 0 SER 22.758 56.988 1.000 21.20 ANISOU 1771 O 260 1917 SER 3689 2448 -75 -269 - 5731772 CB ATOM 260 4.738 SER 21.076 58.480 1.000 20.28 ANISOU 1772 CB SER 260 2491 2458 2755 -101 - 495160 ATOM 1773 OG 260 3.656 SER 20.197 58.227 1.000 22.70 ANISOU 1773 OG SER 260 2758 2574 3294 -113 -284 - 169 261 4.474 ATOM 1774 N SER 23.329 56.330 1.000 18.79 ANISOU 1774 N 261 2189 SER 2215 2737 -55 -92 3 51775 CA ATOM SER 261 4.148 54.929 1.000 16.88 23.585 ANISOU 1775 CA 261 2074 SER 1718 22 -117 -404 2622 ATOM 1776 C SER 261 5.066 22.672 54.106 1.000 17.25 ANISOU 1776 C SER 1833 261 1720 3000 101 -350 - 491ATOM 1777 0 261 6.272 SER 22.876 54.173 1.000 19.96 ANISOU 1777 O 261 1712 2417 SER 3456 50 -483 - 781 1778 CB SER ATOM 261 4.471 25.028 54.503 1.000 19.95 ANISOU 1778 CB SER 261 2903 1675 3002 164 -113 - 1351779 OG ATOM SER 261 4.404 25.127 53.107 1.000 35.64 ANISOU 1779 OG SER 261 5435 4814 3293 -1089 -766 1263 ATOM 1780 N 262 4.467 VAL 53.435 1.000 15.56 21.722 ANISOU 1780 N VAL 262 1751 2140 2021  $-75 \cdot -40 -436$ 1781 CA ATOM VAL 20.713 262 5.247 52.711 1.000 15.41 ANISOU 1781 CA 262 1871 VAL 1938 2048 43 21 - 196 1782 C ATOM VAL 262 4.914 51.242 1.000 14.05 20.874 ANISOU 1782 C VAL 262 1460 1784 2095 -13 29 - 144 ATOM 1783 0 VAL 262 3.759 20.712 50.844 1.000 15.45 ANISOU 1783 O 262 1488 VAL 1900 2481 -175 - 94 - 1911784 CB 262 4.902 ATOM VAL 53.253 1.000 16.87 19.307 ANISOU 1784 CB 262 2144 VAL 2005 2260 165 -164231785 CG1 VAL ATOM 262 5.567 52.364 1.000 20.01 18.275 ANISOU 1785 CG1 VAL 262 2433 3165 2006 4 - 191 - 6371786 CG2 VAL 262 5.335 ATOM 54.715 1.000 18.63 19.200 ANISOU 1786 CG2 VAL 262 2390 2242 2446 -397 1 7 5 147 ATOM 1787 N PHE 263 5.894 50.412 1.000 13.73 21.163 ANISOU 1787 N 263 1497 PHE 1573. 2148 5 -64 1 8 6 1788 CA 263 5.762 ATOM PHE 21.411 48.994 1.000 13.04 ANISOU 1788 CA 263 1654 PHE 1196 2105 -12 -193 1 1 31789 C MOTA PHE 263 6.479 20.253 48.284 1.000 13.56 ANISOU 1789 C PHE 263 1432 1351 2370 -175 -98 -871790 O ATOM PHE 263 7.732 20.177 48.281 1.000 13.83 ANISOU 1790 O PHE 263 1415 1437 2403 -82 -299 - 1041791 CB ATOM PHE 263 6.364 22.770 48.594 1.000 13.50 ANISOU 1791 CB PHE 263 1658 -295 -97 3 4 1374 2098 1792 CG ATOM 263 6.062 PHE 47.135 1.000 13.34 23.148 ANISOU 1792 CG 263 1616 PHE 1358 2096 -159 -111 8 2 ATOM 1793 CD1 PHE 263 6.750 22.635 46.051 1.000 14.95 ANISOU 1793 CD1 PHE 263 1977 -354 -131 - 384 1547 2156 1794 CD2 PHE ATOM 263 5.005 46.883 1.000 15.37 24.048 ANISOU 1794 CD2 PHE 263 1549 1557 -139 -264 3 0 3 2735 1795 CE1 PHE ATOM 263 6.468 22.945 44.720 1.000 14.58 ANISOU 1795 CE1 PHE 263 1721 1621 2196 -242 71 - 144 MOTA 1796 CE2 PHE 263 4.703 45.566 1.000 14.71 24.366 ANISOU 1796 CE2 PHE 263 1482 2680 1428 -20 -261 1 3 7 ATOM 1797 CZ PHE 263 5.383 23.809 44.479 1.000 16.55 ANISOU 1797 CZ PHE 263 1935 1492 -152 2862 29 1 4 ATOM 1798 N 264 5.721 PHE 19.405 47.588 1.000 12.07 ANISOU 1798 N PHE 264 1277 1343 1967 -66 -49 1 9 ATOM 1799 CA PHE 264 6.267 18.328 46.769 1.000 11.90 ANISOU 1799 CA 264 1177 PHE 1289 2058  $-129 \quad 34 \quad -21$ MOTA 1800 C 264 6.440 PHE 18.775 45.314 1.000 11.76

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ANISOU	1800	C	PHE	264	1206	1258	2004	-121 -42 8
ATOM		0	PHE		5.418	19.097	44.683	1.000 12.55
ANISOU		0	PHE		1165	1473	2133	-77 -120 4 6
ATOM		CB	PHE		5.346	17.099	46.773	1.000 12.39
ANISOU	1802		PHE		1101	1498	2110	-304 -42 6 3
ATOM	1803		PHE		5.022	16.558	48.150	1.000 13.97
ANISOU	1803		PHE		1647	1465	2197	-290 13 1 2 1
ATOM ANISOU	1804				5.960	15.848	48.852	1.000 17.07
ATOM	1805				2039 3.747	1976	2471	-422 -410 4 9 7
ANISOU	1805				1835	2359	48.668 2419	1.000 17.41 -440 433 112
ATOM	1806				5.661	15.247	50.053	1.000 20.59
ANISOU	1806	CE1	PHE		2616	2710	2496	-556 -425 7 2 5
ATOM	1807			264	3.458	16.133	49.906	1.000 22.51
ANISOU	1807			264	2151	4047	2355	-787 106 553
ATOM	1808		PHE		4.386	15.350	50.562	1.000 20.88
ANISOU	1808		PHE		2889	2376	2669	-936 -22 3 0 6
ATOM ANISOU		N N	LEU		7.676	18.756	44.811	
ATOM	1810	N C 2	LEU LEU		1192 7.900	1248	2047	-37 47 1 9
	1810		LEU		1264	19.000 1269	43.374	·
ATOM	1811		LEU		7.915	17.617	42.703	
ANISOU	1811	С	LEU		1266	1298		-117 -81 3
ATOM	1812	_	LEU	265	8.842	16.834	42.915	
			LEU		1367	1283	2260	-107 -152 4 4
ATOM	1813		LEU		9.246	19.730	43.156	
ANISOU ATOM	1813		LEU		1399	1364	2019	
ANISOU			LEU LEU		9.500 1168	20.124 1399		
ATOM	1815					21.314	2066 41 318	-292 -248 3 0 2 1.000 13.29
ANISOU					1518	1546	1984	84 36 1 9
MOTA	1816			265	10.971	20.458		1.000 13.14
ANISOU					1204	1593	2197	-234 41 -20
ATOM	1817		ARG			17.249		1.000 12.06
ANISOU ATOM	1817		ARG		1412	1127	2043	
ANISOU			ARG ARG		6.586 1372	15.913 1201		1.000 12.07
ATOM	1819		ARG		6.619	15.965	2012	-258 0 8 0 1.000 11.75
ANISOU	1819		ARG		1203	1315	1948	
ATOM	1820	0	ARG			16.860	39.396	1.000 13.06
ANISOU		0	ARG	266	1430	1318	2214	5 -173 281
ATOM	1821		ARG		5.243	15.370	41.994	1.000 12.95
ANISOU ATOM			ARG		1142	1477	2302	
ANISOU	1822 1822		ARG ARG		5.036 1351	15.606	43.488	
ATOM	1823		ARG		3.723	1686 15.041	2207	-159 66 -115 1.000 12.70
ANISOU			ARG		1369	1362	2094	66 -22 8 4
ATOM	1824		ARG		2.581	15.648		1.000 12.97
ANISOU	1824	•	ARG		1343	1155		52 -165 -137
ATOM	1825				1.304	15.281	43.500	1.000 11.34
ANISOU			_		1432	1009		45 -149 -103
ATOM ANISOU	1826 1826				0.995	14.414	44.476	
ATOM	1827				1802 0.305	1165	2119	
ANISOU					1490	15.821 1067	2210	1.000 12.55 125 -357 -159
ATOM	1828		PRO		7.237	14.951		1.000 12.74
ANISOU			PRO		1418	1394	2030	16 -146 108
ATOM	1829				7.298	14.947		1.000 13.88
ANISOU			PRO		1442	1786	2047	167 -125 - 84
ATOM	1830		PRO		5.957	14.722		1.000 12.61
ANISOU	1830		PRO	267	1413	1508	1868	-6 44 2 7

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- 73 -MOTA 1831 0 PRO 267 4.998 14.155 37.772 1.000 13.60 PRO ANISOU 1831 O 267 1648 1355 2164 -160 118 9 3 1832 CB PRO 267 8.238 ATOM 37.599 1.000 15.30 13.761 ANISOU 1832 CB PRO 267 1435 1740 2637 115 -28 -169 1833 CG MOTA PRO 267 8.033 12.846 38.764 1.000 15.82 ANISOU 1833 CG 267 1885 PRO 1804 2324 381 -270 - 197MOTA 267 7.872 1834 CD PRO 39.965 1.000 14.73 13.746 ANISOU 1834 CD PRO 267 1803 2438 1356 311 -666 - 205 1835 N ATOM ASN 268 5.933 15.051 35.939 1.000 13.27 ANISOU 1835 N 268 1601 ASN 1665 1777 -126 -43 - 1271836 CA MOTA ASN 268 4.800 14.709 35.073 1.000 13.72 ANISOU 1836 CA ASN 268 1793 1401 2018 -214-236 - 711837 C 268 4.723 ATOM ASN 13.192 34.875 1.000 13.14 ANISOU 1837 C 268 1485 ASN 1350 2156 -213104 5 4 1838 0 MOTA ASN 268 5.702 12.467 34.934 1.000 13.90 ANISOU 1838 O ASN 268 1698 1416 2167 123 - 36 -91 1839 CB 268 4.997 15.338 ATOM ASN 33.690 1.000 15.74 ANISOU 1839 CB ASN 268 2597 1369 2016 -437 1 3 5 -66 268 5.011 ASN ATOM 1840 CG 16.862 33.811 1.000 15.41 ANISOU 1840 CG ASN 268 2255 1439 2162 -17 -184471841 OD1 ASN 268 4.069 MOTA 17.454 34.352 1.000 17.75 ANISOU 1841 OD1 ASN 268 2573 1686 2487 42 91 - 98 ATOM 1842 ND2 ASN 268 6.066 17.503 33.319 1.000 16.61 ANISOU 1842 ND2 ASN 268 2408 1355 2546 -50 -57 142 MOTA 1843 N ALA 269 3.531 12.712 34.594 1.000 13.99 ANISOU 1843 N ALA 269 1677 1467 2172 -356 -65 170 1844 CA ALA ATOM 269 3.278 11.286 34.353 1.000 13.42 ANISOU 1844 CA ALA 269 1459 1405 2234 -208 -118 1 0 7 MOTA 1845 C ALA 269 4.182 33.252 1.000 13.93 10.729 ANISOU 1845 C ALA 269 1289 1538 2466 -168 -5 1 5 3, 1846 O ATOM ALA 269 4.581 9.550 33.318 1.000 14.97 ANISOU 1846 O ALA 269 1718 1476 2494 -143112 8 6 ATOM 1847 CB ALA 269 1.806 11.051 34.008 1.000 13.76 ANISOU 1847 CB ALA 1474 269 1300 2454 -60 -61 123 1848 N MOTA ASP 270 4.482 11.541 32.251 1.000 14.38 ANISOU 1848 N 270 1688 ASP 1476. 2300 -15130 - 5 1849 CA MOTA ASP 270 5.247 11.079 31.098 1.000 14.83 ANISOU 1849 CA 270 1747 ASP 1693 2194 -99 -42 6 8 1850 C ATOM ASP 270 6.749 11.287 31.227 1.000 15.68 ASP ANISOU 1850 C 270 1714 1886 2357 8 6 -224 143 ATOM 1851 O ASP 270 7.483 11.008 30.255 1.000 17.12 ANISOU 1851 O ASP 270 1952 2354 2200 -80 139 226 1852 CB ASP ATOM 270 4.718 29.800 1.000 17.67 11.681 ANISOU 1852 CB ASP 270 2461 1966 2288 -75 -319 1 2 6 1853 CG ASP ATOM 270 4.968 13.168 29.649 1.000 18.22 ANISOU 1853 CG ASP 270 2284 2024 2613 -88 -80 474 1854 OD1 ASP ATOM 270 5.386 13.826 30.607 1.000 20.55 ANISOU 1854 OD1 ASP 270 3424 1541 2844 -47 -287425ATOM 1855 OD2 ASP 13.698 270 4.646 28.552 1.000 23.06 ANISOU 1855 OD2 ASP 270 3317 2727 2719 -49 -136 8 1 2 1856 N ATOM PHE 271 7.221 11.668 32.413 1.000 13.93 ANISOU 1856 N PHE 271 1556 1318 2417 97 31 4 1 1857 CA PHE MOTA 271 8.671 11.723 32.644 1.000 14.41 ANISOU 1857 CA 271 1624 PHE 1430 2423 110 29 2 6 3 ATOM 1858 C PHE 271 9.275 10.349 32.325 1.000 13.31 ANISOU 1858 C PHE 271 1402 1430 2225 -30 28 2 1 8 ATOM 1859 0 271 8.790 PHE 9.340 32.870 1.000 14.91 ANISOU 1859 O PHE 271 1900 1374 2392 -26 240 192 ATOM 1860 CB PHE 271 8.942 12.146 34.098 1.000 15.57 ANISOU 1860 CB PHE 271 1700 1721 2495 -66 -36 9 ATOM 1861 CG PHE 271 10.386 11.791 34.516 1.000 14.56

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ANISOU 1861 CG	PHE 271	1729	1320	2485	-152 34 -124
ATOM 1862 CD1		11.460	12.369	33.814	1.000 17.76
ANISOU 1862 CD1	PHE 271	1714	1581	3452	-235 393 -249
ATOM 1863 CD2		10.698	10.972	35.570	1.000 18.04
ANISOU 1863 CD2		2182	1543	3130	-95 -540 1 7 2
ATOM 1864 CE1 ANISOU 1864 CE1		12.786	12.092	34.166	1.000 17.54
ANISOU 1864 CE1 ATOM 1865 CE2	_	1838 11.997	1700	3128	-291 114 - 50
ANISOU 1865 CE2		1935	10.609 1646	35.899 3578	1.000 18.84 -392 -396 4 2 5
ATOM 1866 CZ	_		11.154		-392 -396 4 2 5 1.000 17.25
ANISOU 1866 CZ		2444	1697	2415	-486 -19 -394
ATOM 1867 N		10.278	10.298	31.453	1.000 13.78
ANISOU 1867 N ATOM 1868 CA		1514	1641	2083	30 19 1 5 4
ANISOU 1868 CA		10.811 1551	9.046	30.938	1.000 13.99
ATOM 1869 C	_	12.246	1660 8.841	2105 31.410	-99 83 6 7 1.000 14.71
ANISOU 1869 C		1598	1549	2441	-3 108 3 5 7
ATOM 1870 O		13.046	9.808	31.424	1.000 16.23
ANISOU 1870 O		1646	1742	2780	-246 5 185
ATOM 1871 CB ANISOU 1871 CB		10.751	9.117		1.000 16.27
ATOM 1872 OG1		1856 9.341	2205 9.221	2119 29.032	191 125 8
ANISOU 1872 OG1		1996	2473	23.032	1.000 17.99 64 -190 264
ATOM 1873 CG2	THR 272	11.249	7.856	28.723	1.000 17.94
ANISOU 1873 CG2		2423	2167	2227	173 177 - 9 4
ATOM 1874 N ANISOU 1874 N		12.567 1644	7.600 1521	31.743	1.000 14.91
ATOM 1875 CA		13.894	7.253	2499 32.254	92 238 2 1 8 1.000 15.16
ANISOU 1875 CA		1602	1813	2345	296 277 5 5
ATOM 1876 C		14.350	5.899	31.724	1.000 14.69
ANISOU 1876 C ATOM 1877 O		1408	1647	2528	24 479 1 7 8
ATOM 1877 O ANISOU 1877 O		13.541 1738	5.086 1767	31.262	1.000 15.91
ATOM 1878 CB			7.301	2541 33.769	-115 450 119 1.000 15.77
ANISOU 1878 CB	_	1758	1921	2314	-344 286 123
ATOM 1879 CG		12.931	6.336	34.424	1.000 14.54
ANISOU 1879 CG ATOM 1880 CD1		1390	1726	2410	-95 -11 195
ATOM 1880 CD1 ANISOU 1880 CD1		11.601 1457	6.743 2343	34.655 2521	1.000 16.64 -24 308 362
ATOM 1881 CD2		13.295	5.038	34.721	-24 308 362 1.000 15.23
	PHE 273	1863	1624	2300	-110 91 1 3 6
ATOM 1882 CE1		10.719	5.848	35.259	1.000 16.10
ANISOU 1882 CE1 ATOM 1883 CE2	- · ·	1593	2158	2365	-162 292 122
ANISOU 1883 CE2		12.419 1904	4.148 1980	35.354 2198	1.000 16.01 -139 285 181
ATOM 1884 CZ		11.109	4.559	35.548	1.000 15.18
ANISOU 1884 CZ		1843	2001	1925	-141 73 -227
ATOM 1885 N		15.634	5.612		1.000 15.31
ANISOU 1885 N ATOM 1886 CA		1559	1940	2317	361 383 247
ANISOU 1886 CA		16.221 1476	4.318 1723		1.000 15.37 32 557 156
ATOM 1887 C		15.953			1.000 14.67
ANISOU 1887 C	SER 274	973 187			13 265 3 0 2
ATOM 1888 O		16.310	3.476		1.000 15.98
ANISOU 1888 O ATOM 1889 CB		1668	1677	2728	126 143 193
ANISOU 1889 CB		17.742 1487	4.556 2019	31.356 3112	1.000 17.41 235 945 725
ATOM 1890 OG		18.362	3.280	31.334	
ANISOU 1890 OG	SER 274	1839	1961	3052	293 840 188
ATOM 1891 N		15.395	2.133	32.182	
ANISOU 1891 N	VAL 275	1646	1857	2417	-182 461 261

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> - 75 -ATOM 1892 CA VAL 275 15.158 1.033 33.137 1.000 15.65 ANISOU 1892 CA 275 1681 1800 VAL 2466 -180 261 265 275 16.454 ATOM 1893 C VAL 33.659 1.000 15.33 0.445 ANISOU 1893 C 275 1805 VAL 1881 2139 116 392 - 451894 0 ATOM VAL 275 16.623 0.280 34.871 1.000 15.68 ANISOU 1894 O 275 2037 VAL 1655 2267 6 297 1 9 6 1895 CB ATOM VAL 275 14.227 32.483 1.000 16.05 -0.004ANISOU 1895 CB VAL 275 1635 1708 2755 -76 405 1896 CG1 VAL MOTA 275 14.080 -1.186 33.426 1.000 17.04 ANISOU 1896 CG1 VAL 275 2045 1688 2740 -211 230 1 5 1897 CG2 VAL 275 12.847 MOTA 0.608 32.203 1.000 18.45 275 1650 ANISOU 1897 CG2 VAL 2432 2928 -57 135 1898 N MOTA PRO 0.093 276 17.437 32.844 1.000 16.21 ANISOU 1898 N PRO 276 1927 1700 2532 97 589 3 6 PRO MOTA 1899 CA 276 18.707 33.399 1.000 18.10 -0.434 ANISOU 1899 CA 276 1736 PRO 2115 3025 147 616 - 93276 19.382 MOTA 1900 C PRO 34.321 1.000 17.52 0.541 ANISOU 1900 C PRO 276 1998 1961 2697 97 469 2 3 9 ATOM 1901 0 PRO 276 19.963 0.171 35.348 1.000 19.66 ANISOU 1901 O 276 2015 PRO 2409 3047 24 280 4 6 8 276 19.590 1902 CB MOTA PRO -0.79632.214 1.000 20.80 ANISOU 1902 CB 276 2094 PRO 2687 3121 306 771 - 249ATOM 1903 CG PRO 276 18.852 -0.390 30.999 1.000 21.57 ANISOU 1903 CG 276 2051 PRO 3098 3046 340 802 ATOM 1904 CD PRO 276 17.446 31.368 1.000 18.17 -0.021 ANISOU 1904 CD 276 2053 PRO 2306 2546 179 832 - 318 ATOM 1905 N LEU 277 19.325 1.845 34.027 1.000 17.09 ANISOU 1905 N LEU 277 1571 1898 3025 511 107 230 ATOM 1906 CA 2.802 LEU 277 19.962 34.940 1.000 19.34 ANISOU 1906 CA 277 2035 LEU 2141 3171 -219 218 262 1907 C MOTA LEU 2.858 277 19.214 36.249 1.000 18.34 ANISOU 1907 C 277 1963 LEU 1958 3049 -33 -3 - 3 8 MOTA 1908 0 LEU 277 19.815 2.957 37.319 1.000 19.29 ANISOU 1908 O LEU 277 2466 1710 -271 -188 - 2 3154 ATOM 1909 CB 277 20.094 LEU 34.291 1.000 21.41 4.178 ANISOU 1909 CB LEU 277 2739 2011. 3383 14 12 2 8 7 1910 CG MOTA LEU 277 20.910 5.192 35.111 1.000 26.34 ANISOU 1910 CG 277 3662 LEU 2367 3978 -980 -547 9 4 4 1911 CD1 LEU ATOM 277 22.396 4.839 35.069 1.000 38.04 ANISOU 1911 CD1 LEU 277 3764 3171 7518 -487 -2057 8531912 CD2 LEU 277 20.708 6.607 ATOM 34.631 1.000 31.98 ANISOU 1912 CD2 LEU 277 4023 2018 6109 -366 508 732 ATOM 1913 N 278 17.875 2.711 ALA 36.202 1.000 17.30 ANISOU 1913 N ALA 278 2015 1766 2793 74 218 1 1 5 MOTA 1914 CA ALA 278 17.124 37.464 1.000 16.75 2.712 ANISOU 1914 CA ALA 278 2200 1566 2600 216 146 - 2 1915 C ATOM 278 17.575 ALA 1.523 38.313 1.000 16.31 ANISOU 1915 C ALA 278 1849 1553 -337 -196 1 0 7 2794 ATOM 1916 0 278 17.718 1.635 ALA 39.523 1.000 17.26 ANISOU 1916 O 278 1963 ALA 1839 2754 -53 205 -62 1917 CB MOTA ALA 278 15.642 2.622 37.177 1.000 17.55 ANISOU 1917 CB 278 2109 ALA 1880 2679 295 195 - 11 MOTA 1918 N 279 17.724 0.362 ARG 37.696 1.000 17.07 ANISOU 1918 N 279 2322 ARG 1399 2766 -178 26 3 0 8 MOTA 1919 CA ARG 279 18.099 -0.829 38.473 1.000 16.93 ANISOU 1919 CA 279 2377 ARG 1734 2323 15 -241 203 ATOM 1920 C 279 19.477 -0.587 ARG 39.098 1.000 19.87 ANISOU 1920 C 279 2491 ARG 2292 2766 -487 -384 5 4 3 MOTA 1921 0 279 19.687 -0.974 40.234 1.000 33.04 ARG ANISOU 1921 O ARG 279 3615 4823 -1726 -1700 2603 4115 ATOM 1922 CB 279 18.164 -2.042 37.517 1.000 20.04 ARG

77"

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- 76 -ANISOU 1922 CB ARG 279 2042 1609 3964 108 -221 - 3051923 CG MOTA ARG 279 16.742 -2.49137.179 1.000 20.73 ANISOU 1923 CG ARG 279 2152 2728 2997 -98 -401 - 3511924 CD MOTA ARG 279 16.601 -3.42235.990 1.000 24.81 ANISOU 1924 CD ARG 279 3213 2982 3231 -1 -507 -6091925 NE MOTA 279 17.575 ARG 36.195 1.000 27.50 -4.484ANISOU 1925 NE 279 4331 ARG 2656 3463 355 -146 - 181 MOTA 1926 CZ 279 17.301 -5.725 ARG 36.620 1.000 41.33 279 7720 ANISOU 1926 CZ ARG 5519 2466  $-186 \quad -454 \quad -142$ 1927 NH1 ARG. 279 16.024 -6.012 ATOM 36.866 1.000 40.58 ANISOU 1927 NH1 ARG 279 8821 3012 -1564 507 452 3585 1928 NH2 ARG MOTA -6.688 279 18.200 36.807 1.000 53.27 ANISOU 1928 NH2 ARG 279 9516 2227 8496 -127 -4607 -463 1929 N 280 20.390 MOTA GLU 0.119 38.424 1.000 19.68 ANISOU 1929 N GLU 280 2172 2276 3028 84 324 1 3 6 1930 CA GLU 280 21.748 ATOM 38.948 1.000 20.28 0.334 ANISOU 1930 CA 280 2046 GLU 2274 3385 25 581 1 1 5 1931 C ATOM GLU 280 21.705 40.182 1.000 20.67 1.257 ANISOU 1931 C GLU 280 2334 1968 3552 -281 285 1932 0 ATOM GLU 280 22.723 40.908 1.000 26.81 1.079 ANISOU 1932 O GLU 280 2659 3419 4107 -37 -183 - 87ATOM 1933 CB GLU 280 22.651 1.029 37.926 1.000 24.69 ANISOU 1933 CB GLU 280 2778 2558 4044 1022 3 0 3 -351 ATOM 1934 CG GLU 280 22.997 0.342 36.634 1.000 27.13 ANISOU 1934 CG GLU 280 2605 4888 596 2816 116 623 ATOM 1935 CD 1.298  ${ t GLU}$ 280 23.815 35.760 1.000 43.10 ANISOU 1935 CD 280 4693 GLU 7780 3903 -1328 1206 8 3 4 1936 OE1 GLU ATOM 280 24.541 2.171 36.296 1.000 41.36 ANISOU 1936 OE1 GLU 280 2666 6033 7015 27 1099 690 1937 OE2 GLU 280 23.727 ATOM 1.219 34.520 1.000 64.81 ANISOU 1937 OE2 GLU 280 10844 3751 10028 -2356 1104 2134 CYS ATOM 1938 N 281 20.777 40.313 1.000 21.61 2.156 ANISOU 1938 N CYS 281 2372 2240 3599 -211 532 - 238 ATOM 281 20.481 1939 CA CYS 41.337 1.000 24.33 3.164 ANISOU 1939 CA 281 2114 CYS 2911 4219 -526 1121 - 817 ATOM 1940 C CYS 281 19.858 42.585 1.000 27.11 2.568 ANISOU 1940 C CYS 281 2492 3261 -1608 1457 -1343 4546 ATOM 1941 0 CYS 281 19.789 43.685 1.000 19.19 3.161 ANISOU 1941 O 281 1997 CYS 2012 -250 3282 -326 1 3 5 ATOM 1942 CB 281 19.632 CYS 40.795 1.000 22.02 4.438 ANISOU 1942 CB CYS -286 100 -2108 281 1214 3088 4063 1943 SG MOTA CYS 281 20.639 5.092 39.444 1.000 53.41 ANISOU 1943 SG CYS 281 10822 4742 -3261 1316 4 5 4730 ATOM 1944 N GLY 282 19.370 1.317 42.565 1.000 18.81 ANISOU 1944 N GLY 282 1230 2224 3695 3 - 149 - 2061945 CA ATOM 282 18.675 GLY 0.750 43.744 1.000 17.07 ANISOU 1945 CA 282 1544 GLY 1771 3171 31 -552 -168 1946 C ATOM GLY 282 17.194 43.538 1.000 14.91 0.496 ANISOU 1946 C GLY 282 1601 1645 -135 -453 3 7 8 2417 MOTA 1947 0 GLY 44.380 1.000 16.38 282 16.480 -0.062 ANISOU 1947 O 282 1998 GLY 1921 2306  $-211 \quad -399 \quad 360$ ATOM 1948 N PHE 283 16.625 0.919 42.404 1.000 13.44 ANISOU 1948 N PHE 283 1563 1539 2006  $-189 \quad -336 \quad -115$ 1949 CA ATOM PHE 283 15.173 42.203 1.000 14.52 0.829 ANISOU 1949 CA PHE 283 1677 1410 -187 -670 4 6 2428 1950 C ATOM PHE 283 14.810 -0.604 41.809 1.000 13.08 ANISOU 1950 C PHE 283 1519 -121 -338 1 7 4 1314 2137 1951 0 ATOM PHE 283 15.311 40.837 1.000 14.11 -1.184 ANISOU 1951 O PHE 283 1366 1418 -142 -78 1 7 2578 1952 CB ATOM 283 14.749 PHE 1.800 41.078 1.000 13.76 ANISOU 1952 CB PHE 283 1814 1288 2125 -39 -2680

- 77 -ATOM 1953 CG PHE 283 14.842 3.269 41.512 1.000 14.75 ANISOU 1953 CG PHE 283 1985 1363 2255 12 - 317 - 31954 CD1 PHE ATOM 283 13.814 3.904 42.142 1.000 21.50 ANISOU 1954 CD1 PHE 283 2318 1759 4091 -23 -626 303 1955 CD2 PHE ATOM 283 15.994 3.999 41.298 1.000 17.72 ANISOU 1955 CD2 PHE 283 2526 1244 2963 -89 272 -307 1956 CE1 PHE 283 13.909 ATOM 5.177 42.655 1.000 20.78 ANISOU 1956 CE1 PHE 283 2056 ' 1802 4036 92 66.-647 1957 CE2 PHE 283 16.115 ATOM 5.290 41.814 1.000 15.06 ANISOU 1957 CE2 PHE 283 2101 1257 -5 -255 2364 3 7 7 1958 CZ 283 15.084 ATOM PHE 5.891 42.506 1.000 18.04 ANISOU 1958 CZ PHE 283 1881 1995 2979 192 -432 2 0 MOTA 1959 N ASP 284 13.883 -1.17842.579 1.000 13.07 ANISOU 1959 N ASP 1366 284 1549 2049 -73 -331 1 1 7 ATOM 1960 CA ASP 284 13.502 -2.584 42.395 1.000 12.80 ANISOU 1960 CA 284 1481 ASP 1460 1924 -231 -207 1 5 7 284 12.335 ATOM 1961 C ASP -2.65441.421 1.000 12.88 284 1493 ANISOU 1961 C ASP 1508 1891 -19 -180 - 55MOTA 1962 0 284 11.231 ASP -3.14741.741 1.000 13.69 ANISOU 1962 O ASP 284 1407 1351 2442 -281 9 2 -93 MOTA 1963 CB ASP 284 13.141 43.744 1.000 14.10 -3.203ANISOU 1963 CB ASP 284 1966 1534 1858 -40-11 145 MOTA 1964 CG ASP 284 13.165 -4.73043.717 1.000 14.49 ANISOU 1964 CG ASP 284 1906 1520 2079 47 -424 290 1965 OD1 ASP MOTA 284 13.732 42.758 1.000 14.81 -5.305 ANISOU 1965 OD1 ASP 284 2036 1343 2250 -152 -166 2 3 1 1966 OD2 ASP 284 12.652 ATOM -5.310 44.696 1.000 15.32 ANISOU 1966 OD2 ASP 1557 284:1979 -79 2286 -109 1 5 3 285 12.644 ATOM 1967 N VAL 40.217 1.000 12.40 -2.191ANISOU 1967 N 285 1582 VAL 1870 1260 79 -185 -131 ATOM 1968 CA VAL 285 11.599 39.216 1.000 12.31 -2.064ANISOU 1968 CA 285 1442 VAL 1469 1767 -161 - 59 - 11969 C ATOM 285 11.229 VAL 38.589 1.000 12.09 -3.419ANISOU 1969 C VAL 285 1220 1407 1967 -1 -100 -79ATOM 1970 0 VAL 285 12.085 38.433 1.000 13.68 -4.311ANISOU 1970 O 285 1237 VAL 1514 2446 67 56 4 0 285 12.009 MOTA 1971 CB VAL -1.066 38.098 1.000 14.68 ANISOU 1971 CB VAL 285 1943 1621 -163 -50 259 2014 1972 CG1 VAL 285 12.131 ATOM 0.332 38.672 1.000 17.08 ANISOU 1972 CG1 VAL 285 2429 1402 2658 18 -465 425 ATOM 1973 CG2 VAL 285 13.309 -1.499 37.433 1.000 15.69 ANISOU 1973 CG2 VAL 285 2131 2180 -316 161 3 0 6 1649 1974 N SER ATOM 286 9.952 -3.541 38.241 1.000 12.24 ANISOU 1974 N SER 286 1263 1440 1946 -12 -148 - 117MOTA 1975 CA 286 9.398 SER -4.669 37.495 1.000 12.84 ANISOU 1975 CA 286 1571 SER 1463 1845 -356 -30 1 4 MOTA 1976 C 286 8.861 SER 36.172 1.000 11.99 -4.118ANISOU 1976 C SER 286 1516 1374 1666 -28 60 - 198 ATOM 1977 O SER 286 7.654 -4.110 35.917 1.000 15.68 ANISOU 1977 O SER 286 1514 2384 2059 2 18 - 20 1978 CB ATOM SER -5.327 286 8.301 38.300 1.000 12.54 ANISOU 1978 CB 286 1407 SER 1442 1915 -59 170 - 55 ATOM 1979 OG SER 286 7.415 -4.38038.890 1.000 13.15 ANISOU 1979 OG SER 286 1531 1430 -73 - 5 9 2034 105 MOTA 1980 N LEU 287 9.769 -3.649 35.333 1.000 13.56 ANISOU 1980 N 287 1574 LEU 1521 2058 41 133 1 7 7 1981 CA LEU ATOM 287 9.451 -2.932 34.101 1.000 13.48 ANISOU 1981 CA 287 1812 LEU 1418 1891 -84 116 1 7 1982 C ATOM 287 10.075 -3.654 LEU 32.908 1.000 15.12 ANISOU 1982 C 287 1945 1714 LEU 2086 32 233 - 3 1 MOTA 1983 0 287 11.277 -3.883 LEU 32.927 1.000 17.91

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291 11.695 MOTA 2014 OG1 THR 3.862 27.077 1.000 25.98 ANISOU 2014 OG1 THR 291 3160 4072 2641 -86 703 503 MOTA 2015 CG2 THR 291 14.048 27.292 1.000 24.20 4.115 291 3199 ANISOU 2015 CG2 THR 3832 2164 930 533 -445 ATOM 2016 N 292 10.959 ALA 3.658 30.492 1.000 14.84 ANISOU 2016 N ALA 292 1637 1656 2347 200 429 - 153 2017 CA MOTA ALA 292 9.675 31.179 1.000 13.84 3.657 292 1488 ANISOU 2017 CA ALA 1477 2294 170 299 7 8 ATOM 2018 C ALA 292 9.356 31.619 1.000 12.65 5.065 ALA ANISOU 2018 C 292 1334 1564 1908 60 144 - 139 ATOM 2019 0 ALA 292 10.228 31.710 1.000 14.27 5.939 ANISOU 2019 O ALA 292 1529 1596 2295 -35 109 116 ATOM 2020 CB ALA 292 9.670 32.414 1.000 14.02 2.754 ANISOU 2020 CB ALA 292 1693 37 22 - 27 1580 2053 ATOM 2021 N THR 293 8.054 5.258 31.916 1.000 13.54 ANISOU 2021 N 293 1468 THR 1617 · 2058 117 373 -118 293 7.605 ATOM 2022 CA THR 6.546 32.424 1.000 13.40 ANISOU 2022 CA THR 293 1565 1647 1877 152 209 - 232 ATOM 2023 C THR 293 7.407 6.482 33.952 1.000 12.09 ANISOU 2023 C 293 1345 THR 1322 1927 -62 326 - 12ATOM 2024 O THR 293 7.214 34.555 1.000 12.93 5.441 ANISOU 2024 O THR 293 1385 1356 2170 -190 194 9 0 293 6.295 ATOM 2025 CB THR 31.788 1.000 13.45 7.058 ANISOU 2025 CB THR 293 1598 1579 1935 95 345 3 4 5 2026 OG1 THR ATOM 293 5.273 32.117 1.000 13.75 6.112 ANISOU 2026 OG1 THR 293 1672 1570 1981 -12 314 1 3 5 ATOM 2027 CG2 THR 293 6.476 30.272 1.000 15.93 7.139 ANISOU 2027 CG2 THR 293 2121 2022 1911 255 434 337 ATOM 294 7.241 2028 N PHE 34.544 1.000 12.81 7.661 ANISOU 2028 N PHE 294 1607 1440 1822 -83 149 -151 ATOM 2029 CA PHE 294 6.857 7.773 35.935 1.000 12.37 ANISOU 2029 CA PHE 294 1332 1469 1899 -267 166 - 289 MOTA 2030 C PHE 294 5.556 36.184 1.000 12.36 7.022 ANISOU 2030 C PHE 294 1336 1361 1999 -151 30 - 36MOTA 2031 0 PHE 294 5.403 6.253 37.143 1.000 13.27 ANISOU 2031 O PHE 2076 294 1556 1410 -191 183 4 6 ATOM 2032 CB PHE 294 6.698 36.267 1.000 13.83 9.271 ANISOU 2032 CB PHE 294 2039 1351 1866 -192 -29 -177 294 6.306 ATOM 2033 CG PHE 9.488 37.711 1.000 13.10 ANISOU 2033 CG PHE 294 1786 1216 1974 -125 -63 -244 2034 CD1 PHE ATOM 294 7.207 38.749 1.000 17.41 9.411 ANISOU 2034 CD1 PHE 294 2132 2533 1952 -1012 -287 7 6 ATOM 294 4.964 2035 CD2 PHE 38.026 1.000 18.41 9.739 ANISOU 2035 CD2 PHE 294 2156 2263 2575 565 332 2036 CE1 PHE ATOM 294 6.810 9.608 40.054 1.00@ 17.72 ANISOU 2036 CE1 PHE 294 2348 2296 2086 -308 -362 -136 2037 CE2 PHE MOTA 294 4.591 39.324 1.000 19.37 10.010 ANISOU 2037 CE2 PHE 294 2078 2541 2740 330 232 - 630 MOTA 2038 CZ PHE 294 5.507 40.355 1.000 18.36 9.956 ANISOU 2038 CZ PHE 294 2443 1678 -394 -55 -2452855 ATOM 2039 N 7.205 GLN 295 4.588 35.246 1.000 12.59 ANISOU 2039 N GLN 295 1248 1429 2106 -62 38 - 168 ATOM 2040 CA GLN 295 3.320 35.408 1.000 12.76 6.484 ANISOU 2040 CA GLN 295 1266 1215 2365 7 -157 -117 ATOM 2041 C GLN 295 3.512 4.984 35.318 1.000 12.24 ANISOU 2041 C 295 1449 GLN 1256 1944 10 1 - 7 3 MOTA 295 2.922 2042 0 GLN 4.238 36.101 1.000 13.61 ANISOU 2042 O GLN 295 1323 1427 7 85 1 5 5 2424 ATOM 2043 CB GLN 295 2.375 6.975 34.317 1.000 14.31 ANISOU 2043 CB GLN 295 1227 1594 81 -133 192 2616 ATOM 2044 CG GLN 295 1.062 6.256 34.249 1.000 14.03

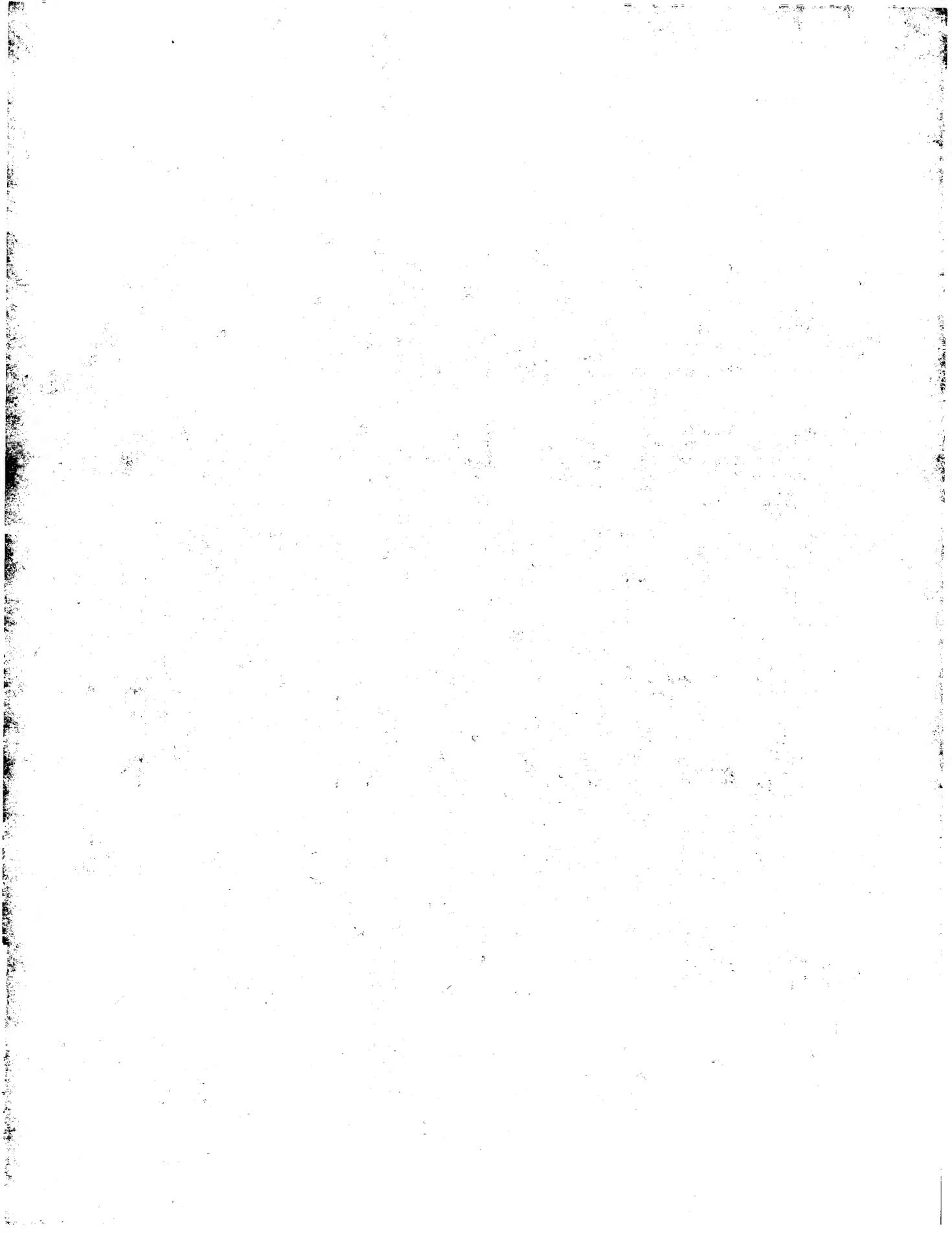
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ANISOU	2044	CG	GLN	295	1391	- 80 -	2420	5.0 2.00 4.5	5.0 2.00 4.5
ATOM	2045		GLN		0.157	1509 5.687	2430	-59 -300 4 7	
ANISOU	2045		GLN		1305	1486	2361	1.000 13.56 133 -117 165	
ATOM	2046				0.459	7.693		1.000 15.35	
ANISOU					1811	1651	2371	161 206 220	
ATOM	2047				-0.982	6.026		1.000 15.04	
ANISOU	2047	NE2	GLN	295	1225	1995	2493	75 -139 - 99	
ATOM	2048		ASP	296	4.363	4.463		1.000 12.66	
ANISOU			ASP		1425	1396	1990	181 -112 - 110	
ATOM	2049		ASP		4.653	3.016	34.439	1.000 12.26	_
ANISOU	2049		ASP		1628	1274	1755	53 -51 - 151	
ATOM	2050	_	ASP		5.167	2.569		1.000 11.57	.000 11.57
ANISOU ATOM	2050 2051	_	ASP		1199	1300	1895	-82 30 - 22	
ANISOU	2051		ASP ASP		4.854 1534	1.460		1.000 13.08	
ATOM	2052		ASP		5.709	1368 2.634	2070	-107 38 1 3 9	
ANISOU			ASP		1870	1700	1819	1.000 14.18	
ATOM	2053		ASP		5.295	2.848		141 30 - 378 1.000 13.32	
ANISOU			ASP		1655	1557	1848	-58 67 2	
ATOM	2054	OD1	ASP		4.110	2.725		1.000 15.83	
ANISOU				296	1680	1935	2402	-68 -126 - 189	
ATOM	2055				6.212	3.098		1.000 15.27	
ANISOU	2055				1757	1937	2106	-229 137 177	
ATOM	2056		TRP		6.038	3.352		1.000 12.26	
ANISOU ATOM	2056 2057		TRP		1325	1403	1931		
ANISOU			TRP		6.683	2.960		1.000 12.82	
ATOM	2058		TRP TRP		1328 5.746	1599	1943		•
ANISOU			TRP		1418	3.007 1580		1.000 13.13	
ATOM	2059		TRP		5.565	2.030		24 -23 1 8 5 1.000 14.03	
ANISOU		_	TRP		1554	1619	2159		
ATOM	2060	СВ	TRP		7.908			1.000 13.68	
ANISOU			TRP		1130	1692	2376		
ATOM	2061		TRP		8.646	3.455		1.000 13.28	
ANISOU			TRP		1143	1646	2255	91 -96 2 2	91 -96 2 2
ATOM	2062				8.932		39.622	1.000 15.58	1.000 15.58
ANISOU					1615	1689	2618	275 -544 - 77	
ATOM ANISOU	2063				9.144			1.000 14.69	
ATOM	2064				1327 9.583	· · · · ·	2562		
ANISOU					1378	2.265 1853		1.000 15.34	
ATOM	2065				9.724	3.597		70 -494 7 5 1.000 16.13	
ANISOU					1241		2880		
ATOM	2066	CE3	TRP		9.094	_		1.000 22.13	
ANISOU					3040	1658	3712		-
MOTA			TRP	297	10.318	4.180		1.000 18.45	- <del>-</del>
ANISOU					2204	2387		44 -326 -331	•
ATOM			TRP		9.670		41.399	1.000 21.55	1.000 21.55
ANISOU					2916		3167		
ATOM ANISOU			TRP		10.258			1.000 23.53	
ATOM	2070		ILE		3298	2356	3285	-320 -1146 -34	
ANISOU			ILE		5.106 1324	4.167		1.000 13.58	
ATOM	2071		ILE		4.299	1726 4.440		241 -167 1 2 7 1.000 14.68	
ANISOU			ILE		1413	2177	1986		
ATOM	2072		ILE		2.841	4.054		1.000 12.02	
ANISOU			ILE		1455	1300	1813		
ATOM	2073		ILE	298	2.182			1.000 13.67	
ANISOU			ILE		1732	1582	1881		
ATOM	2074		ILE		4.428	5.914	40.673	1.000 19.45	
ANISOU	20/4	CB	ILE	298	2261	2446	2683	-699 237 -835	-699 237 -835

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MOTA 2075 CG1 ILE 298 5.907 6.245 41.001 1.000 27.83 ANISOU 2075 CG1 ILE 4275 298 2776 3525 -1314 -556 -1030 2076 CG2 ILE MOTA 6.319 298 3.679 41.929 1.000 25.05 ANISOU 2076 CG2 ILE 298 3770 3344 2405 -57 255 - 983 2077 CD1 ILE MOTA 298 6.368 5.628 42.306 1.000 43.32 ANISOU 2077 CD1 ILE 298 4561 7224 4674 -652 -1890 -117 ATOM 2078 N GLY 299 2.317 3.980 38.893 1.000 12.16 ANISOU 2078 N 1308 GLY 299 1432 78 -304 106 1879 MOTA 2079 CA GLY 38.670 1.000 12.98 299 0.918 3.741 ANISOU 2079 CA GLY 299 1276 1279 2379 106 -188 - 154299 0.135 ATOM 2080 C GLY 38.378 1.000 13.09 5.017 ANISOU 2080 C GLY 299 1421 1403 2151 113 -231 1 1 8 **ATOM** 2081 0 GLY 299 0.738 6.025 38.017 1.000 14.00 ANISOU 2081 O GLY 299 1713 1353 2252 122 289 - 13 MOTA 2082 N GLY 300 -1.183 38.447 1.000 13.08 4.917 ANISOU 2082 N GLY 300 1325 1545 2099 146 -267 - 145ATOM 2083 CA GLY 300 - 2.0755.966 37.992 1.000 13.45 ANISOU 2083 CA GLY 300 1447 1521 -415 -143 2143 116 GLY ATOM 2084 C 300 - 2.5196.972 39.042 1.000 12.94 ANISOU 2084 C GLY 300 1098 1365 2456 -52 -407 - 192MOTA 2085 O GLY 300 - 3.2627.875 38.672 1.000 13.39 ANISOU 2085 O GLY 300 1321 1342 2423 -19 -217 - 45ATOM 2086 N ASN 40.254 1.000 13.35 301 -1.973 6.845 ANISOU 2086 N ASN 301 1494 1429 2151 -225 -232 - 104ATOM 2087 CA ASN 7.842 301 -2.162 41.313 1.000 13.83 ANISOU 2087 CA ASN 301 1590 1435 -194 -38 -61 2230 ATOM 2088 C ASN 41.885 1.000 12.46 301 -0.837 8.254 ANISOU 2088 C ASN 301 1676 1268 1791 -35-142 - 20ATOM 2089 O ASN 42.169 1.000 13.89 301 -0.007 7.405 ANISOU 2089 O ASN 301 1831 1355 2093 73 - 144 - 13ATOM 2090 CB ASN 301 -3.075 7.238 42.360 1.000 16.01 ANISOU 2090 CB ASN 1909 301 1632 2542 77 224 3 1 5 MOTA 2091 CG ASN 301 - 3.9428.199 43.106 1.000 18.23 ANISOU 2091 CG ASN 301 1986 2435 2508 190 152 - 90ATOM 2092 OD1 ASN 42.614 1.000 17.44 301 -4.973 8.690 ANISOU 2092 OD1 ASN 301 1606 1626 3394 -21 144 - 190 ATOM 2093 ND2 ASN 301 -3.518 8.454 44.338 1.000 33.30 ANISOU 2093 ND2 ASN 6923 301 2804 2928 -230 -1523 1012 ATOM 2094 N TYR 302 -0.595 9.564 42.073 1.000 12.96 ANISOU 2094 N TYR 302 1662 1278 1985 -69 -21 - 135MOTA 2095 CA TYR 42.702 1.000 13.48 302 0.674 9.948 ANISOU 2095 CA TYR 302 1673 1259 2192 -130 -132 3 4 ATOM 2096 C TYR 44.078 1.000 12.63 302 0.768 9.269 ANISOU 2096 C TYR 302 1413 1293 2092 53 44 1 9 MOTA 2097 0 TYR 302 -0.218 9.151 44.806 1.000 14.15 ANISOU 2097 O TYR 302 1332 1737 2305 -65 48 - 272098 CB MOTA TYR 302 0.764 42.916 1.000 13.30 11.472 ANISOU 2098 CB TYR 302 1635 1192 2226 -81 33 4 1 ATOM 2099 CG TYR 302 1.159 12.143 41.619 1.000 12.02 ANISOU 2099 CG TYR 302 1586 1880 1103 -59 -25 . - 271 302 2.501 ATOM 2100 CD1 TYR 12.233 41.275 1.000 13.11 ANISOU 2100 CD1 TYR 302 1633 1284 2066 11 - 18 -80 ATOM 2101 CD2 TYR 302 0.235 12.709 40.739 1.000 12.52 ANISOU 2101 CD2 TYR 302 1576 1132 2049 -44 13 - 127 MOTA 2102 CE1 TYR 40.119 1.000 12.29 302 2.933 12.822 ANISOU 2102 CE1 TYR 302-1581 1043 -185 -84 -7.72045 2103 CE2 TYR ATOM 302 0.637 13.273 39.535 1.000 14.12 ANISOU 2103 CE2 TYR 302 1462 1443 2458 -241 15 3 2 5 ATOM 2104 CZ 39.241 1.000 12.69 TYR 302 1.983 13.347 ANISOU 2104 CZ 302 1483 TYR 1224 2113 -287 -91 1 0 MOTA 2105 OH TYR 302 2.376 13.866 38.013 1.000 13.42



- 82 -ANISOU 2105 OH TYR 302 1505 1469 -93 2124 33 146 MOTA 2106 N VAL 303 1.956 8.855 44.450 1.000 13.92 ANISOU 2106 N VAL 303 1406 1637 2246 153 88 9 9 2107 CA ATOM VAL 303 2.355 8.336 45.746 1.000 14.51 ANISOU 2107 CA VAL 303 1838 -391 - 741320 2355 -137 MOTA 2108 C VAL 303 3.498 9.244 46.239 1.000 15.23 ANISOU 2108 C VAL 303 1404 1507 2876 -102 -105 - 348MOTA 2109 0 VAL 303 4.471 45.512 1.000 18.70 9.386 VAL ANISOU 2109 O 303 1859 1861 3386 -239 326 -504 MOTA 2110 CB VAL 45.632 1.000 16.75 303 2.856 6.880 ANISOU 2110 CB VAL 303 2140 1319 2905 16 -759 -123 ATOM 2111 CG1 VAL 303 3.279 6.401 47.017 1.000 19.53 ANISOU 2111 CG1 VAL 303 2185 1951 3284 232 -1054 148 2112 CG2 VAL 45.125 1.000 17.82 ATOM 303 1.723 5.956 ANISOU 2112 CG2 VAL 303 2476 1442 -213 2852 -558 - 406 2113 N MOTA ASN 304 3.349 47.378 1.000 14.07 9.900 ANISOU 2113 N ASN 304 1409 1369 2566 -39 -407 - 86304 4.317 ATOM 2114 CA ASN 10.928 47.772 1.000 14.31 ANISOU 2114 CA ASN 304 1474 1387 2578 -102 -424 -552115 C ATOM ASN 304 5.450 10.397 48.637 1.000 13.75 ANISOU 2115 C ASN 304 1360 1487 2378 34 -274 - 87 2116 O 48.584 1.000 14.60 MOTA ASN 304 6.539 10.962 ANISOU 2116 O ASN 304 1314 1795 2438 -34 -55 -320 MOTA 2117 CB ASN 304 3.589 12.035 48.551 1.000 14.26 ANISOU 2117 CB ASN 304 1710 1214 2494 6 -303 176 2118 CG MOTA ASN 304 2.535 12.661 47.642 1.000 14.81 ANISOU 2118 CG ASN 304 1551 1627 2449 23 -114 402 304 2.866 2119 OD1 ASN ATOM 13.255 46.622 1.000 16.52 ANISOU 2119 OD1 ASN 304 1896 1746 2636 80 19 5 8 9 MOTA 2120 ND2 ASN 304 1.290 12.595 48.102 1.000 18.43 ANISOU 2120 ND2 ASN 2980 304 1560 2463 127 -10 199 ATOM 2121 N ILE 305 5.175 9.413 49.463 1.000 16.36 ANISOU 2121 N ILE 305 1546 1553 3117 -78 -503 2 6 6 ATOM 2122 CA ILE 305 6.173 8.890 50.407 1.000 14.85 ANISOU 2122 CA ILE 305 1670 165 1537 2436 -277 - 40ATOM 2123 C 305 6.183 ILE 7.372 50.352 1.000 15.78 ANISOU 2123 C ILE 305 1527 1555 2914 95 -438 -51 MOTA 2124 0 ILE 305 5.231 6.736 49.886 1.000 17.54 ANISOU 2124 O ILE 305 1463 1789 3412 -131 -4045MOTA 2125 CB ILE 305 5.949 51.818 1.000 17.80 9.430 ANISOU 2125 CB ILE 305 2167 1962 2634 -23 265 - 209MOTA 2126 CG1 ILE 305 4.578 9.091 52.416 1.000 18.93 ANISOU 2126 CG1 ILE 305 1716 2948 2526 1 -218 -163 2127 CG2 ILE 305 6.171 ATOM 10.944 51.823 1.000 19.17 ANISOU 2127 CG2 ILE 70 - 534 - 405 305 2685 1863 2737 2128 CD1 ILE MOTA 305 4.415 9.459 53.863 1.000 21.28 ANISOU 2128 CD1 ILE 305 2521 2902 2662 19 452 - 71 2129 N MOTA ARG 306 7.246 6.806 50.908 1.000 14.59 ANISOU 2129 N 306 1738 ARG 1641 2165 52 -356 271 MOTA 2130 CA ARG 306 7.424 5.360 50.828 1.000 15.25 ANISOU 2130 CA ARG 1663 306 1509 2622 139 -302 7 7 MOTA 2131 C ARG 306 8.234 52.024 1.000 15.02 4.903 ANISOU 2131 C ARG 306 1588 1464 2656 133 -332 - 21MOTA 2132 0 ARG 306 9.141 52.433 1.000 16.63 5.614 ANISOU 2132 O ARG 306 1682 2101 2536 -219 -294 -168 ATOM 2133 CB ARG 306 8.135 4.943 49.532 1.000 16.31 ANISOU 2133 CB 306 1820 ARG 1681 2697 -100 -270 -150MOTA 2134 CG ARG 306 8.226 49.377 1.000 18.43 3.414 ANISOU 2134 CG ARG 306 2476 1700 2828 40 - 194 - 156 3.068 ATOM 2135 CD ARG 306 8.401 47.900 1.000 18.26 ANISOU 2135 CD ARG 306 2087 1971 2880  $-120 \quad -145 \quad -330$ 

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ATOM	2136	ME	ARG	306	7.136	3 220	47 100	1 000	20 72
						3.228	47.188		
ANISOU			ARG		2442	2013	3345	-577	-668 -234
ATOM	2137		ARG	306	6.980	3.178	45.873	1.000	20.27
ANISOU	2137	CZ	ARG	306	2330	2057	3316	373	-522 2 0
MOTA	2138	NH1			8.086				
						3.000	45.107	1.000	22.13
ANISOU		-	ARG		2136	2580	3695	274	-589 - 723
ATOM	2139	NH2	ARG	306	5.759	3.250	45.341	1.000	18.44
ANISOU	2139	NH2	ARG	306	2107	1838	3062	259	
ATOM	2140		ARG		7.898				-285 8 4
						3.775	52.612	1.000	19.10
ANISOU			ARG		2716	1872	2671	-294	-607 3 2 7
ATOM	2141	CA	ARG	307	8.576	3.212	53.768	1.000	21.13
ANISOU	2141	CA	ARG		3321 -	2201	2504		
ATOM	2142		ARG		· · · -	· <del>-</del>		-48	-845 1 3 9
					9.536	2.138	53.277	1.000	23.30
ANISOU	2142		ARG	307	3417	2170	3267	181	-1046 3 9
ATOM	2143	0	ARG	307	9.385	1.601	52.187	1.000	
ANISOU	2143	0	ARG		2574	2355	3052		
ATOM	2144							174	-728 1 1 2
			ARG		7.557	2.522	54.694	1.000	27.30
ANISOU	2144	_	ARG	307	4545	3184	2645	-13	-247 7 0 5
ATOM	2145	CG	ARG	307	6.839	3.488	55.629	1.000	46.30
ANISOU	2145	CG	ARG		6310	6374	4907		
ATOM	2146							215	1655 - 970
			ARG		7.054	3.085	57.085	1.000	66.50
ANISOU	2146	CD	ARG		11107	10355	3806	-2980	2792 - 1145
ATOM	2147	NE	ARG	307	5.989	2.203	57.531	1.000	78.91
ANISOU	2147	NE	ARG		11821	12833	5330		1969 - 5
ATOM					5.987				
						1.285			
ANISOU			ARG		7704	14382	5907	-4724	1249 1051
$\mathtt{ATOM}$				307	7.063	1.038	59.214	1,000	80.32
ANISOU	2149	NH1	ARG		6613		5955		2179 1 0 5
ATOM					4.872				
							58.707		
ANISOU					9116		2983	-6954	438 - 917
ATOM	2151	N	THR	308	10.551	1.861	54.113	1.000	25.61
ANISOU	2151	N	THR		4234	2212			-1421 - 232
ATOM			THR		11.308				
ANISOU							53.822		
			THR		3468	1939	5998	225	-1629 - 194
$\mathtt{ATOM}$	2153	C	THR	308	10.468	-0.611	54.030	1.000	25.42
ANISOU	2153	С	THR	308	2915	2190	4552		
ATOM	2154	0	THR		9.523	·			
ANISOU						-0.768			
			THR		4042	3482	3912		-217 -125
ATOM	2155		THR	308	12.581	0.531	54.688	1.000	26.09
ANISOU	2155	CB	THR	308	2701	3586	3626	242	-361 - 456
ATOM	2156	0G1	THR		12.140				
ANISOU	2156	001	mun						
					4146	4188	4167		
ATOM	2157	CGZ	THR		13.577	1.594	54.256	1.000	31.43
ANISOU	2157	CG2	THR	308	3193	4702	4047	-577	-132 -538
ATOM	2158	N	SER	309	10.850				
ANISOU			SER		2934				
									74 - 391
ATOM	2159				10.199				
ANISOU	2159	CA	SER	309	3793	2464	3316	-485	451 - 230
ATOM	2160	С	SER	309	10.466	-3.691	54.512		
ANISOU	2160	C	SER		2360				
ATOM		_				2888	3893	302	107 3 5
	2161		SER		11.565	-3.621	55.084	1.000	34.54
ANISOU		_	SER	309	3626	2131	7366	-76	-1944 - 34
MOTA	2162	CB	SER	309	10.639	-3.700	52.012		
ANISOU			SER		3970				
ATOM	2163					2159	3948		
			SER		10.217	-5.039	52.148	1.000	26.34
ANISOU			SER	309	3198	2207	4604	156	-844 - 260
ATOM	2164	N	LYS	310	9.494	-4.458	54.961		
ANISOU	2164	N	LYS		3172	2459			
ATOM	2165						3864	160	262 366
			LYS		9.651	-5.339	56.125		28.38
ANISOU			LYS		4191	3167	3427	764	278 281
ATOM	2166	С	LYS	310	9.941	-6.768		-	26.07
					- <del>-</del>				~ ~ . ~ .

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ANISOU	2166 C		310	3371	2687	3846	168	-290 5 7 7
$\mathtt{ATOM}$	2167 0		310	10.150	-7.684	56.515	1.000	33.48
ANISOU	2167 0	LYS	310	5267	3056	4400	-66	-450 1073
ATOM	2168 CB	LYS	310	8.299	-5.367	56.858	1.000	37.77
ANISOU	2168 CB	LYS	310	5736	4695	3921	299	1818 1 8
ATOM	2169 CG	LYS	310	8.014	-4.214		1.000	40.55
ANISOU	2169 CG	LYS	310	6395	4716	4295	1525	1524 1 0 1
ATOM	2170 CD	LYS	310	6.798	-4.537		1.000	44.24
ANISOU	2170 CD	LYS	310	9091	4224	3495	1053	2816 5 8 4
ATOM	2171 CE	LYS	310	6.722	-6.109	58.818	1.000	
ANISOU	2171 CE	LYS	310	9281	4577	8606	766	-82 2478
ATOM	2172 NZ	LYS	310	6.088	-6.563	60.089		55.80
ANISOU	2172 NZ	LYS	310	4884	5742	10577	287	-947 4796
ATOM	2173 N			9.896	-7.030	54.410	1.000	22.45
ANISOU	2173 N	ALA	311	2190	2402	3939	10 52	2 6 9
ATOM	2174 CA	ALA	311	10.360	-8.369	53.972	1.000	31.89
ANISOU	2174 CA			3771	2594	5753	434	-516 -421
ATOM	2175 C		311		-8.459	53.833	1.000	23.30
ANISOU	2175 C			3907	2328	2616	1393	-593 1 1 2
ATOM	2176 CB		311	· · - <del>-</del> -	-8.665	52.674	1.000	27.94
ANISOU	2176 CB		311		2878	5329	-355	542 - 672
ATOM	2177 OW			-6.477	10.237	44.256		15.66
ATOM	2178 OW			-9.349	<del>-</del>	51.010		
MOTA	2179 OW			-1.489	3.653	34.560		
ATOM	2180 OW 2181 OW			-10.499		50.182		
ATOM ATOM				-8.612	16.958	47.640		
ATOM	2182 OW 2183 OW			-10.255		42.881		
ATOM	2184 OW			2.096 -0.284	1.076	32.810		
ATOM	2185 OW			-8.525		41.885		13.93
ATOM	2186 OW			3.165	2.604	42.416 43.488		
ATOM	2187 OW			-6.282	19.386	52.341		
ATOM	2188 OW			-6.826	24.638	46.833		
ATOM	2189 OW			10.510	-4.344	46.092		
ATOM	2190 OW			-0.806	16.964	40.372		
ATOM	2191 OW			-1.269	18.855	42.411		
ATOM	2192 OW		516		-5.146	40.175		
ATOM	2193 OW	HOH	517	-0.123	21.538	40.640		
MOTA	2194 OW	HOH	518	13.131	-0.967	51.791		
ATOM	2195 OW	HOH	519	11.009	2.875	45.599	1.000	20.20
ATOM	2196 OW	HOH	520	5.789	13.543	45.996	1.000	17.36
ATOM	2197 OW	HOH		2.168	19.767	55.925	1.000	20.41
ATOM	2198 OW	HOH		8.487	15.960	34.949	1.000	15.40
MOTA	2199 OW	НОН	523		12.697			19.99
MOTA	2200 OW	нон		-11.722				19.82
ATOM	2201 OW	нон		1.672	-2.081			16.29
ATOM	2202 OW	НОН		9.651	15.283			20.37
ATOM	2203 OW	НОН		28.749	31.187			18.53
ATOM ATOM	2204 OW	НОН		15.326				19.60
ATOM	2205 OW 2206 OW	НОН		26.897	26.984			19.86
ATOM	2206 OW 2207 OW	HOH		13.528	11.592			
ATOM	2207 OW 2208 OW	НОН		25.631	32.409	52.682		
ATOM	2208 OW 2209 OW	HOH		18.287	6.835	52.185		
ATOM	2210 OW	HOH HOH		12.635				
ATOM	2210 OW 2211 OW	HOH		10.797				20.66
ATOM	2211 OW 2212 OW	HOH		10.167 23.530				19.12
ATOM	2212 OW 2213 OW	HOH		23.358	24.122			20.39
ATOM	2213 OW 2214 OW	HOH		25.879	12.639			22.61
ATOM	2214 OW 2215 OW	HOH		11.674	28.699			19.44
ATOM	2215 OW 2216 OW	НОН		18.515	16.559 27.775			18.57
	2210 OW	поп	J # ()	T0.3T3	21.115	40.042	1.000	22.23

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ATOM 2217 OW 541 21.233 HOH 20.367 33.996 1.000 21.45 ATOM 2218 OW 542 22.826 53.094 1.000 19.38 HOH 32.643 ATOM 2219 OW 543 19.670 35.310 1.000 20.05 HOH 22.387 2220 OW 544 -13.591 21.996 ATOM HOH 61.494 1.000 49.93 2221 OW ATOM HOH 545 21.295 11.783 55.080 1.000 20.04 2222 OW ATOM HOH 546 5.431 2.533 51.677 1.000 28.11 2223 OW ATOM HOH 547 17.311 25.489 32.148 1.000 24.38 2224 OW HOH 548 17.427 ATOM 7.744 33.008 1.000 20.78 ATOM 2225 OW HOH 23.874 549 11.656 58.194 1.000 23.39 2226 OW MOTA HOH 550 8.037 14.987 53.326 1.000 33.52 2227 OW ATOM 14.574 551 1.354 33.889 1.000 21.05 HOH 552 11.203 2228 OW MOTA 63.686 1.000 24.59 HOH 20.116 2229 OW ATOM HOH 553 2.671 21.240 34.245 1.000 34.51 ATOM 2230 OW HOH 554 6.339 30.751 1.000 26.36 19.832 2231 OW ATOM HOH 555 26.611 24.519 55.570 1.000 21.22 2232 OW ATOM HOH 556 27.669 17.156 53.039 1.000 25.86 2233 OW ATOM HOH 557 -14.392 19.977 44.154 1.000 25.03 2234 OW 558 14.828 MOTA HOH 32.652 51.443 1.000 25.23 ATOM 2235 OW HOH 559 17.937 7.207 54.915 1.000 20.59 ATOM 2236 OW -8.875 HOH 560 10.729 31.499 1.000 24.65 ATOM 2237 OW HOH 561 6.455 2.298 42.613 1.000 22.74 2238 OW ATOM HOH 562 13.784 31.245 44.166 1.000 27.75 2239 OW ATOM 563 17.292 HOH 33.470 53.556 1.000 25.28 ATOM 2240 OW HOH 564 11.210 1.109 49.697 1.000 23.33 2241 OW ATOM HOH 565 -11.339 25.246 41.370 1.000 26.08 2242 OW ATOM HOH 566 20.363 -8.37538.242 1.000 30.07 2243 OW ATOM 24.604 HOH 567 3.890 35.837 1.000 25.86 MOTA 2244 OW HOH 568 5.334 43.937 1.000 25.45 11.875 2245 OW ATOM 569 7.861 HOH 22.385 64.046 1.000 28.98 ATOM 2246 OW -1.508 HOH 570 7.754 30.848 1.000 24.72 ATOM 2247 OW 571 6.297 28.471 1.000 33.06 HOH 3.583 ATOM 2248 OW HOH 572 -15.790 28.800 51.855 1.000 30.09 ATOM 2249 OW HOH 573 -5.388 20.310 38.883 1.000 23.64 574 17.657 ATOM 2250 OW 21.059 HOH 29.053 1.000 24.31 2251 OW ATOM HOH 20.920 66.102 1.000 24.81 575 8.763 2252 OW ATOM 576 10.135 HOH 27.617 58.357 1.000 25.12 2253 OW ATOM HOH 1.060 577 7.795 29.730 1.000 29.00 ATOM 2254 OW 578 22.601 HOH 19.580 61.946 1.000 28.66 ATOM 2255 OW HOH 579 8.859 4.744 27.898 1.000 26.12 2256 OW ATOM 48.882 1.000 26.29 HOH 580 4.937 3.932 35.057 1.000 23.31 581 17.096 ATOM 2257 OW HOH 5.891 MOTA 2258 OW HOH 582 -16.337 31.047 64.719 1.000 54.01 ATOM 2259 OW 583 7.652 HOH 24.826 52.106 1.000 27.23 2260 OW MOTA HOH 584 7.174 24.915 29.292 1.000 26.60 ATOM 2261 OW HOH 585 23.452 10.614 55.439 1.000 26.42 ATOM 2262 OW HOH 586 12.640 26.413 58.676 1.000 27.15 ATOM 2263 OW HOH 587 6.204 21.166 62.094 1.000 24.65 2264 OW ATOM HOH 588 2.385 0.810 37.616 1.000 19.92 ATOM 2265 OW 589 32.930 HOH 28.236 45.738 1.000 38.29 ATOM 2266 OW HOH 590 -12.045 28.716 45.065 1.000 30.46 ATOM 2267 OW HOH 591 0.219 13.612 36.120 1.000 27.12 2268 OW ATOM HOH 592 -2.525 3.881 43.344 1.000 26.67 ATOM 2269 OW HOH 593 7.533 13.297 48.055 1.000 19.59 ATOM 2270 OW 594 -1.575 HOH 28.355 42.057 1.000 25.53 ATOM 2271 OW HOH 595 11.209 -1.188 46.425 1.000 22.12 ATOM 2272 OW 596 5..684 HOH -7.000 28.451 1.000 27.97 2273 OW MOTA HOH 597 28.868 19.406 51.825 1.000 27.72 ATOM 2274 OW 598 13.432 HOH 2.493 57.904 1.000 31.12 2275 OW ATOM 599 8.196 HOH 7.483 27.148 1.000 29.99 ATOM 2276 OW 600 20.809 19.088 HOH 63.369 1.000 36.86 ATOM 2277 OW 601 21.352 HOH 10.656 34.614 1.000 30.60

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ATOM	2278 OW	HOH	602 2.891	7.196	30.899 1.000 25.41
ATOM	2279 OW	HOH	603 8.260	26.496	34.561 1.000 35.71
ATOM	2280 OW	НОН	604 22.300	13.959	31.378 1.000 32.53
ATOM ATOM	2281 OW 2282 OW	HOH	605 15.689	35.750	48.870 1.000 31.17
ATOM	2282 OW 2283 OW	НОН НОН	606 7.219 607 -3.237	15.638	30.914 1.000 27.80
ATOM	2284 OW	НОН	608 17.543	14.604 10.581	47.092 1.000 20.96
ATOM	2285 OW	нон	609 -1.899	36.370	33.561 1.000 23.51 44.261 1.000 32.64
ATOM	2286 OW	HOH	610 26.095	14.431	43.803 1.000 19.19
ATOM	2287 OW	HOH	611 27.664	13.183	41.954 1.000 26.48
ATOM ATOM	2288 OW 2289 OW	НОН	612 4.302	34.604	49.981 1.000 24.70
ATOM	2289 OW 2290 OW	HOH HOH	613 -15.580 614 1.615		46.728 1.000 42.45
ATOM	2291 OW	нон	615 -10.137	35.544 34.259	50.347 1.000 23.78 49.033 1.000 23.94
ATOM	2292 OW	HOH	616 26.084	6.502	49.033 1.000 23.94 57.657 1.000 39.32
ATOM	2293 OW	HOH	617 -15.962	20.656	46.340 1.000 25.94
ATOM	2294 OW	HOH	618 6.113	29.517	40.143 1.000 29.43
ATOM ATOM	2295 OW 2296 OW	HOH HOH	619 19.797	4.627	51.313 1.000 27.15
ATOM	2290 OW 2297 OW	HOH	620 -1.748 621 11.099	11.315 34.289	48.716 1.000 21.83
ATOM	2298 OW	НОН	622 28.352	14.351	44.259 1.000 27.15 37.877 1.000 41.48
ATOM	2299 OW	HOH	623 -2.826	36.968	57.149 1.000 32.75
ATOM.	2300 OW	нон	624 16.983	9.258	29.962 1.000 32.82
ATOM ATOM	2301 OW 2302 OW	HOH HOH	625 16.780	29.213	38.384 1.000 27.96
ATOM	2302 OW	HOH	626 1.632 627 33.536	17.213 23.640	33.689 1.000 23.17
ATOM	2304 OW	нон	628 23.821	6.059	45.028 1.000 41.91 50.174 1.000 34.22
ATOM	2305 OW	HOH	629 3.482	2.785	46.751 1.000 39.07
ATOM	2306 OW	НОН	630 20.218	24.803	60.918 1.000 50.12
ATOM ATOM	2307 OW 2308 OW	HOH	631 3.366	16.272	30.698 1.000 31.50
ATOM	2308 OW 2309 OW	HOH HOH	632 18.871 633 4.455	11.791 25.782	31.384 1.000 30.78
ATOM	2310 OW	НОН	634 24.721	5.202	58.823 1.000 32.14 40.319 1.000 40.13
MOTA	2311 OW	HOH	635 19.623	35.238	43.466 1.000 50.48
ATOM	2312 OW	НОН	636 22.789	26.242	60.797 1.000 26.58
ATOM ATOM	2313 OW 2314 OW	HOH	637 7.008	-4.809	54.039 1.000 33.89
ATOM	2314 OW 2315 OW	HOH HOH	638 -15.821 639 -11.847	18.362	42.559 1.000 29.61
ATOM	2316 OW	нон	640 -1.948	13.411	52.841 1.000 25.21 35.401 1.000 30.41
ATOM	2317 OW	HOH	641 -14.293	21.937	42.145 1.000 27.58
ATOM	2318 OW	нон	642 18.216	20.839	66.863 1.000 31.23
ATOM ATOM	2319 OW 2320 OW	HOH	643 9.836	36.288	48.178 1.000 44.21
ATOM	2320 OW 2321 OW	HOH HOH	644 3.510 645 7.571	16.168	66.253 1.000 33.82
ATOM	2322 OW	HOH	646 0.780	33.398 21.844	41.687 1.000 37.96 36.729 1.000 31.71
ATOM	2323 OW	HOH	647 21.244	-2.321	35.579 1.000 32.40
ATOM	2324 OW	НОН	648 3.027	25.244	69.907 1.000 36.84
ATOM ATOM	2325 OW 2326 OW	HOH	649 1.129	25.273	66.516 1.000 35.42
ATOM	2327 OW	нон нон	650 14.646 651 <b>-</b> 8.287	7.560	60.327 1.000 46.42
ATOM	2328 OW	HOH	652 10.153	26.381 23.548	37.998 1.000 29.17 67.703 1.000 31.50
ATOM	2329 OW	нон	653 28.906	22.258	38.969 1.000 32.66
ATOM	2330 OW	нон	654 13.568	-4.482	31.517 1.000 26.94
ATOM ATOM	2331 OW 2332 OW	HOH	655 -12.635	17.106	55.637 1.000 26.85
ATOM	2332 OW 2333 OW	HOH	656 2.698 657 -1.384	5.770	50.702 1.000 29.05
ATOM	2333 OW	HOH	658 3.880	7.487 19.246	46.512 1.000 36.52 31.498 1.000 31.50
ATOM	2335 OW	нон		31.406	64.001 1.000 56.62
ATOM	2336 OW	нон	660 11.416	23.260	65.229 1.000 32.69
ATOM	2337 OW	HOH	661 15.994	14.673	25.680 1.000 36.46
ATOM	2338 OW	нон	662 28.572	21.242	53.423 1.000 39.06

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ATOM 2339 OW HOH 663 19.354 0.465 27.273 1.000 44.56 ATOM 2340 OW HOH 664 24.969 27.026 38.838 1.000 35.41 ATOM HOH 2341 OW 665 24.294 7.488 55.914 1.000 32.97 ATOM 2342 OW HOH 666 19.540 7.882 31.178 1.000 30.04 ATOM 2343 OW HOH 32.988 667 -9.236 57.241 1.000 39.20 2344 OW ATOM HOH 668 2.098 18.351 67.496 1.000 38.88 ATOM 2345 OW HOH 669 11.390 3.245 56.270 1.000 37.56 ATOM 2346 OW HOH 670 -21.413 24.449 52.026 1.000 44.66 ATOM 2347 OW 671 -14.575 19.220 · HOH 55.240 1.000 30.91 ATOM 2348 OW HOH 672 32.112 25.958 43.051 1.000 33.34 673 -15.050 31.151 2349 OW MOTA HOH 53.232 1.000 34.71 2350 OW ATOM HOH 674 2.941 -1.607 30.245 1.000 34.63 2351 OW 14.544 ATOM HOH 675 26.951 34.757 1.000 49.17 ATOM 2352 OW 676 14.707 HOH 30.669 39.386 1.000 30.55 ATOM 2353 OW HOH 677 5.203 18.009 68.080 1.000 43.41 ATOM 2354 OW HOH 678 14.151 7.965 26.591 1.000 38.80 ATOM 2355 OW 679 24.470 HOH 24.261 41.443 1.000 31.28 ATOM 2356 OW HOH 680 17.540 2.410 28.478 1.000 34.31 2357 OW ATOM HOH 681 25.992 20.593 34.326 1.000 39.66 ATOM 2358 OW HOH 682 13.802 35.357 44.421 1.000 34.06 2359 OW ATOM HOH 683 1.087 2.355 45.456 1.000 35.39 ATOM 2360 OW HOH 684 22.443 34.538 42.053 1.000 33.55 ATOM 2361 OW HOH 685 4.419 4.720 27.356 1.000 48.02 ATOM 2362 OW HOH 686 -15.830 34.507 51.877 1.000 50.63 ATOM 2363 OW HOH 687 -15.217 29.490 48.887 1.000 33.54 ATOM 2364 OW HOH 688 36.808 21.183 46.206 1.000 44.97 ATOM 2365 OW HOH 689 3.756 1.312 29.272 1.000 35.16 ATOM 2366 OW 690 18.802 HOH 27.901 1.000 30.08 13.646 ATOM 2367 OW HOH 691 6.997 17.521 29.313 1.000 47.70 ATOM 2368 OW 692 13.725 HOH 16.327 69.105 1.000 36.97 2369 OW ATOM HOH 693 22.369 22.161 60.503 1.000 44.09 ATOM 2370 OW HOH 694 - 5.42942.219 1.000 33.40 31.620 ATOM 2371 OW HOH 695 19.351 30.744 1.000 34.21 23.082 2372 OW ATOM HOH 696 6.897 22.414 29.376 1.000 36.59 2373 OW ATOM HOH 697 28.700 7.809 57.304 1.000 38.35 2374 OW ATOM 698 3.224 HOH 0.679 39.819 1.000 24.13 MOTA 2375 OW HOH 699 -4.634 33.717 62.593 1.000 32.26 ATOM 2376 OW HOH 700 32.423 43.200 1.000 43.20 17.018 ATOM 2377 OW HOH 701 12.119 25.228 68.342 1.000 39.95 702 9.307 ATOM 2378 OW HOH 16.477 28.976 1.000 31.75 2379 OW HOH ATOM 703 -11.313 34.067 46.117 1.000 49.40 2380 OW ATOM HOH 704 7.774 65.371 1.000 39.12 31.390 ATOM 2381 OW HOH 705 24.764 7.530 36.802 1.000 38.55 ATOM 2382 OW 706 -22.095 25.669 59.047 1.000 36.71 HOH ATOM 2383 OW HOH 707 14.509 9.840 68.854 1.000 50.38 ATOM 2384 OW 708 -10.129 28.722 HOH 42.036 1.000 38.92 ATOM 2385 OW HOH 34.910 48.390 1.000 35.29 709 29.011 ATOM 2386 OW 710 15.822 HOH 31.612 42.021 1.000 33.61 ATOM 2387 OW HOH 711 -1.996 17.676 33.645 1.000 49.57 ATOM 2388 OW HOH 712 10.216 17.748 26.015 1.000 41.04 ATOM 2389 OW HOH 713 23.535 37.371 1.000 43.47 29.642 2390 OW ATOM HOH 714 20.488 -7.21435.599 1.000 45.99 2391 OW ATOM HOH 715 11.411 10.149 25.081 1.000 41.63 2392 OW ATOM 716 19.329 -4.258 HOH 34.139 1.000 42.50 ATOM 2393 OW 717 13.688 HOH 26.799 66.321 1.000 43.74 ATOM 2394 OW HOH 718 -10.751 33.064 54.747 1.000 40.47 2395 OW ATOM 719 13.800 HOH 18.258 70.756 1.000 34.54 ATOM 2396 OW HOH 720 17.151 5.815 28.003 1.000 40.80 ATOM 2397 OW HOH 721 0.000 0.000 36.691 0.330 27.42 ATOM 2398 OW HOH 722 0.000 0.000 41.559 0.330 37.77 ATOM 2399 OW 723 15.314 7.549 HOH 28.791 1.000 36.24 **4**)

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2400 OW MOTA HOH 19.944 724 -1.663 39.196 1.000 33.87 ATOM 2401 OW HOH 725 19.289 24.195 33.321 1.000 32.28 ATOM 2402 OW HOH 726 0.000 0.000 31.798 0.330 50.38 2403 OW ATOM HOH 727 -1.223 38.165 59.229 1.000 31.24 728 22.035 ATOM 2404 OW HOH 38.254 45.742 1.000 48.21 ATOM 2405 OW HOH 729 28.388 16.248 63.044 1.000 31.59 ATOM 2406 OW HOH 730 0.000 0.000 45.995 0.330 36.14 ATOM 2407 OW HOH 731 2.984 29.007 40.091 1.000 36.08 2408 MOTA HOH OW 732 5.297 15.835 27.318 1.000 41.53 733 17.347 ATOM 2409 OW HOH 10.778 27.373 1.000 35.27 ATOM 2410 OW HOH 734 29.417 14.607 53.127 1.000 40.12 MOTA 2411 OW HOH 735 4.222 27.012 1.000 35.22 -8.636 MOTA 2412 OW HOH 736 -9.949 17.712 62.813 1.000 34.43 2413 OW ATOM HOH -10.203 55.259 1.000 31.79 737 13.960 2414 OW ATOM HOH 738 11.831 -1.522 49.308 1.000 25.22 2415 OW MOTA HOH 739 2.896 4.247 29.596 1.000 38.64 2416 OW MOTA HOH 740 10.959 25.528 13.759 1.000 61.86 MOTA 2417 OW HOH 741 0.864 17.227 30.557 1.000 50.71 2418 MOTA HOH OW 742 31.755 18.949 52.065 1.000 40.48 ATOM 2419 OW HOH 28.218 1.000 43.23 743 21.678 -0.485 2420 OW ATOM HOH 744 10.583 16.397 75.211 1.000 45.04 ATOM 2421 OW 78.287 1.000 57.64 HOH 745 7.480 7.996 MOTA 2422 OW HOH 746 24.067 35.122 40.297 1.000 41.95 ATOM 2423 OW HOH 747 7.804 10.269 78.332 1.000 49.63 MOTA 2424 OW HOH 748 22.131 40.645 45.806 1.000 49.69 ATOM 2425 HOH OW -4.647 33.872 1.000 42.88 749 14.850 ATOM 2426 OW HOH 32.504 55.211 1.000 37.15 750 -12.930 MOTA 2427 OW HOH 751 -4.832 35.986 43.333 1.000 44.39 2428 ATOM HOH 752 19.834 1.000 31.56 OW 33.566 56.449 MOTA 2429 OW 22.310 HOH 753 3.363 29.844 1.000 42.02 ATOM 2430 OW HOH 754 25.594 4.030 34.174 1.000 51.90 ATOM 2431 OW HOH 755 28.036 46.448 1.000 39.50 35.859 ATOM 2432 OW 756 -12.951 HOH 16.294 61.787 1.000 40.94 MOTA HOH 757 -10.870 2433 OW 26.452 38.737 1.000 44.85 MOTA 2434 OW HOH 758 13.216 12.896 70.729 1.000 63.42 MOTA 2435 OW HOH 759 -0.403 74.990 1.000 38.96 21.161 ATOM 2436 OW HOH 32.526 64.316 1.000 39.64 760 -7.025 MOTA 2437 OW HOH 19.739 58.090 1.000 40.84 761 -15.459 ATOM . 2438 OW HOH 762 -4.964 36.577 59.068 1.000 48.64 MOTA 2439 OW 763 26.807 HOH 35.717 50.036 1.000 43.54 MOTA 2440 OW HOH 7.083 65.538 1.000 41.41 764 19.542 **ATOM** HOH 42.709 1.000 33.78 2441 OW 765 3.709 35.837 33.688 ATOM 2442 OW HOH 40.172 1.000 36.91 766 0.431 ATOM 2443 OW HOH 767 18.620 5.064 64.617 1.000 45.76 MOTA 2444 OW HOH 768 35.526 19.792 41.322 1.000 52.54 MOTA 2445 OW HOH 769 19.671 7.789 67.717 1.000 43.44 MOTA 2446 OW HOH 770 3.562 12.048 26.149 1.000 40.08 MOTA 2447 OW HOH 35.637 53.927 1.000 52.16 771 20.245 MOTA 2448 OW HOH 25.640 61.573 1.000 58.60 772 -20.588 ATOM HOH 2449 OW 773 1.556 37.342 52.171 1.000 36.23 ATOM 2450 OW HOH 49.382 1.000107.24 0.668 774 8.340 MOTA 2451 OW 34.466 1.000 59.84 HOH 775 27.160 2.372 ATOM 2452 OW HOH 776 6.575 19.271 25.545 1.000 36.68

MOTA	2453	OW	HOH	777	-17.605	29.205	62.661	1.000	56.83
ATOM	2454	OW	НОН	778	7.616	6.902	24.722	1.000	61.34
MOTA	2455	OW	HOH	779	19.749	10.700	68.006	1.000	65.22
ATOM	2456	M	НОН	780	7.281	-5.270	50.090	1.000	50.00
ATOM	2457	W	НОН	781	-6.809	28.483	40.515	1.000	50.00
ATOM	2458	W	нон	782	9.990	17.263	38.636	1.000	50.00
ATOM	2459	W	HOH	783	5.767	-2.331	28.939	1.000	50.00
MOTA	2460	W	HOH	784	11.694	-0.118	24.984	1.000	50.00
MOTA	2461	W	HOH	785	24.442	7.952	47.994	1.000	50.00
MOTA	2462	W	HOH	786	14.251	36.889	46.491	1.000	50.00
ATOM	2463	W	HOH	787	5.759	26.477	33.851	1.000	50.00
ATOM	2464	W	HOH	788	-11.816	22.606	40.795	1.000	50.00
ATOM	2465	W	HOH	789	-2.531	5.579	45.829	1.000	50.00
ATOM	2466	W	HOH	790	-13.002	32.034	46.612	1.000	50.00
ATOM	2467	W	HOH	791	2.230	3.555	48.985	1.000	50.00
ATOM	2468	W	HOH	792	9.397	13.464	28.121	1.000	50.00
ATOM	2469	W	HOH	793	28.257	10.442	42.781	1.000	50.00
ATOM	2470	W	НОН	794	4.652	17.944	59.241	1.000	50.00
ATOM	2471	W	HOH	795	5.977	15.287	79.554	1.000	50.00
ATOM	2472	W	НОН	796	30.501	11.852	47.616	1.000	50.00
ATOM	2473	W	HOH	797	5.625	14.258	54.367	1.000	50.00
ATOM	2474	W	HOH	798	23.942	20.228	33.277	1.000	50.00
MOTA	2475	W	HOH	799	10.164	14.642	58.997	1.000	50.00
MOTA	2476	W	HOH	80Õ	7.807	31.943	52.999	1.000	50.00
ATOM	2477	W	HOH	801	23.377	9.361	34.817	1.000	50.00
ATOM	2478	W	HOH	802	21.193	9.722	32.004	1.000	50.00
ATOM	2479	M	HOH	803	34.928	14.644	46.038	1.000	50.00
ATOM	2480	W	HOH	804	29.073	16.684	34.445	1.000	50.00
ATOM	2481	W	HOH	805	7.008	-2.049	51.872	1.000	50.00
ATOM	2482	W	HOH	806	25.363	7.860	45.531	1.000	50.00
ATOM	2483	W	HOH	807	30.704	8.207	55.971	1.000	50.00
ATOM	2484	W	HOH	808	33.072	24.900	40.599	1.000	50.00
ATOM	2485	W	HOH	809	-15.577	19.225	63.152	1.000	50.00
ATOM	2486	W	HOH	810	6.072	18.137	23.603	1.000	50.00
ATOM	2487	W	HOH	811	-7.214	39.940	55.639	1.000	50.00
ATOM	2488	W	HOH	812	5.509	18.517	74.919	1.000	50.00
MOTA	2489	W	HOH	813	33.845	9.908	56.672	1.000	50.00
ATOM	2490	W	HOH	814	0.421	35.779	42.931	1.000	50.00
ATOM.	2491	W	HOH	815	35.282	21.705	48.656	1.000	50.00
ATOM	2492	M .	HOH	816	39.344	22.173	46.871	1.000	50.00
ATOM	2493	W	НОН	817	-5.192	39.820	60.056	1.000	50.00
ATOM	2494	W	НОН	818	30.199	13.039	33.383	1.000	50.00
ATOM	2495	W	НОН	819	-4.860	36.454	61.731	1.000	50.00
ATOM	2496	W	НОН	820	-14.599	17.407	58.382	1.000	50.00
ATOM	2497	W	НОН	821	1.340	-0.111	41.711	0.500	50.00
ATOM	2498	W	НОН	822	34.512	23.218	52.108	1.000	50.00
ATOM	2499	W	НОН	823	32.136	12.571	52.190	1.000	50.00
ATOM	2500	W	НОН	824	13.525	-6.549	29.838	1.000	50.00
MOTA	2501	W	НОН	825	6.072	-4.141	27.534	1.000	50.00

## STRUCTURE B

ATOM 1 ANISOU 1	CB CB	MET MET	1 1	31.030 5663	11.882 3892	57.066 9809	1.000 50.96 1113 -2217 -554
ATOM 2	CG	MET	1	30.206	12.690	56.086	1.000 51.63
ANISOU 2 ATOM 3	CG	MET MET	1 1	6595 28.694	3775 11.848	92 <sup>-</sup> 46 55.559	691 -1891 1 6 9 1.000 4 0 . 5 0
ATOM 3 ANISOU 3	SD SD	MET	1	7003	3962	4424	833 -1535 - 460
ATOM 4	CE	MET	1	27.852	11.584	57.120	1.000 45.32
ANISOU 4	CE	MET	1	8632	3912.	4677	-239 -653 -1702
ATOM 5 ANISOU 5	C C	MET MET	1 1	31.587 6204	13.367 4752	58.999 8854	1.000 52.14 287 -2128 - 63
ATOM 6	0	MET	1	31.239	12.847	60.058	1.000 52.92
ANISOU 6	0	MET	1	7381	5242	7483	1417 -4224 5 1 9
ATOM 7	N	MET	1	33.170	11.646	58.275	1.000 57.78
ANISOU 7 ATOM 8 '	N CA	MET MET	1 1	4533 32.156	6034 12.587	11388 57.819	34 -1912 -811 1.000 54.62
ANISOU 8	CA	MET	1	6441	4752	9560	137 -2012 -617
ATOM 9	N	ASP	2	31.485	14.679	58.792	1.000 43.52
ANISOU 9 ATOM 10	N CA	ASP ASP	2 2	3460 30.759	4866 15.471	8210 59.796	474 -2350 4 7 1.000 41.69
ATOM 10 ANISOU 10	CA	ASP	2	4439	4678	6722	-309 -2603 - 31
ATOM 11	CB	ASP	2	31.206	16.912	59.644	1.000 37.89
ANISOU 11	CB	ASP	2	3805	4768	5822	-304 -3473 266
ATOM 12 ANISOU 12	CG CG	ASP ASP	2	30.219 4511	17.958 4616	60.121 5916	1.000 39.59 15 -3218 589
ATOM 13		ASP	2	29.325		60.933	1.000 45.10
ANISOU 13		ASP	2	5866	4689	6581	-553 -1950 -625
ATOM 14			2	30.363	19.121	59.663	1.000 42.05 -465 -3788 1 4 5
ANISOU 14 ATOM 15	OD2 C	ASP ASP	2 2	5994 29.275	4341 15.213	5643 59.556	-465 -3788 1 4 5 1.000 3 3 . 8 4
ANISOU 15	Ċ	ASP	2	4131	3634	5094	-59 -1682 -122
ATOM 16	0	ASP	2	28.901	15.176	58.379	1.000 29.25
ANISOU 16 ATOM 17	O N	ASP THR	2 3	2232 28.467	4393 15.029	4489 60.597	658 -390 - 615 1.000 29.41
ANISOU 17	N	THR	3	4731	2636	3807	907 -2076 - 284
ATOM 18	CA	THR	3	27.046	14.764	60.421	1.000 28.55
ANISOU 18	CA	THR	3	4602	2494	3753	597 -1006 - 390
ATOM 19 ANISOU 19	CB CB	THR THR	3 3	26.447 7170	13.762 2209	61.414 4495	1.000 36.51 -791 -1996 5 2
ATOM 20	OG1	THR	3	26.629	14.220	62.758	1.000 42.45
ANISOU 20	OG1	THR	3	9519	2620	3989	-920 -1251 3 8 3
ATOM 21	CG2	THR	3	27.153	12.412	61.315	1.000 50.26 -602 -733 -333
ANISOU 21 ATOM 22	CG2 C	THR THR	3 3	9604 26.240	1863 16.061	7630 60.553	1.000 29.01
ANISOU 22	Č	THR	3	4535	2548	3939	738 -1079 9 9
ATOM 23	0	THR	3	25.041	16.044	60.827	1.000 35.82
ANISOU 23 ATOM 24	O N	THR	3	5149	2485	5976 60.332	390 524 -1246 1.000 24.98
ATOM 24 ANISOU 24	N N	THR THR	4 4	26.928 3874	17.181 2456	3162	542 -2040 - 986
ATOM 25	CA	THR	4	26.214	18.465	60.327	
ANISOU 25	CA	THR	4	3437	2426	3244	344 -1563 - 375
ATOM 26 ANISOU 26	CB	THR THR	4 4	27.183 2636	19.650 2429	60.408 5105	1.000 26.77 651 -988 -923
ATOM 27	CB OG1		4	28.050	19.484	61.551	1.000 32.62
ANISOU 27		THR	4	3398	2812	6184	195 -2081 -1134
ATOM 28	CG2		4	26.429	20.942	60.663	1.000 26.40
ANISOU 28 ATOM 29	CG2	THR THR	4 4	2373 25.325	2692 18.577	4967 59.097	533 -573 -1570 1.000 21.64
ANISOU 29	C	THR	4	3090	2760	2374	368 -750 - 2 0
ATOM 30	0	THR	4	25.738	18.264	57.980	1.000 21.58
ANISOU 30	0	THR	4	2668	2629	2902	246 -560 -659
ATOM 31	N	VAL	5	24.104	19.049	59.340	1.000 15.88

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ANISOU 31 ATOM 32 ANISOU 32 ANISOU 33 ANISOU 34 ANISOU 35 ANISOU 35 ANISOU 36 ANISOU 37 ANISOU 37 ANISOU 37 ANISOU 39 ANISOU 40 ANISOU 40 ANISOU 41 ANISOU 41 ANISOU 42 ANISOU 42 ANISOU 42 ANISOU 42 ANISOU 43 ANISOU 44 ANISOU 44 ANISOU 44 ANISOU 45 ANISOU 46 ANISOU 46 ANISOU 47 ANISOU 47 ANISOU 47 ANISOU 47 ANISOU 48 ANISOU 49 ANISOU 49 ANISOU 49 ANISOU 49 ANISOU 49 ANISOU 51 ANISOU 51 ANISOU 51 ANISOU 51 ANISOU 53 ANISOU 57 ANISOU 57 ANISOU 57 ANISOU 57 ANISOU 57	VALLULLU OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO	777777777778888888888888888888888888888	2505 23.211 2463 21.742 2476 20.855 24.68 21.310 23.63 23.63 23.63 23.66 24.667 23.88 24.667 23.88 23.571 23.88 24.048 23.121 23.298 23.299 23.2	2133	1998 55.799 1905 56.998 1858 55.261 2513 53.539 2212 53.600 2738 52.472 1919 51.283 1971 50.067 2025 50.258 2257 50.628 2329	-613 -630 - 162 1.000 14.80 -594 -473 - 87 1.000 16.09 -412 -406 5 0 2 1.000 14.91 9 -102 197 1.000 21.15 -700 -418 1198 1.000 17.70 -1137 -713 1 0 3 1.000 17.35 -698 -650 1 0 5 1.000 13.23 -162 -668 4 0 9 1.000 15.56 -309 -383 2 7 7 1.000 14.49 -218 -536 5 2 2 1.000 18.21 -224 130 4 3 4 1.000 20.37 -1078 38 - 6 1 1.000 14.59 -406 -786 6 9 8 1.000 13.06 -283 -596 1 5 1.000 14.56 -380 -565 5 8 7 1.000 14.56 -380 -565 5 8 7 1.000 14.44 -348 -1257 3 2 9 1.000 14.44 -348 -1257 3 2 9 1.000 14.44 -348 -1257 3 2 9 1.000 14.98 -213 -727 4 1 2 1.000 14.98 -213 -727 4 1 2 1.000 14.98 -213 -727 4 1 2 1.000 14.62 -355 -693 7 0 4 1.000 17.21 -641 -840 9 7 5 1.000 12.32 -314 -534 3 7 0 1.000 13.31 -60 -295 3 4 3 1.000 13.71 -136 -232 2 3 4 1.000 13.68 -185 8 1 5 5 1.000 14.10 -93 231 2 1 1.000 17.52 -234 -56 9 1 7
ANISOU 55 ATOM 56 ANISOU 56 ATOM 57	CG PHE CD1 PHE CD1 PHE CD2 PHE	8 8 8	24.635 1225 24.147 1317 26.006	24.746 1716 23.503 1710 24.882	50.258 2257 50.628 2329 50.079 3134 50.812 2497 50.271 3301 50.654 2757	1.000 13.68 -185 8 155 1.000 14.10 -93 231 221 1.000 17.52 -234 -56 917 1.000 15.39 -11 242 481 1.000 17.73 -157 -143 423

ATOM PHE 62 21.602 28.033 0 51.079 1.000 13.18 ANISOU 62 0 PHE 8 1392 1295 2322 -256 -400364ATOM 63 SER 23.478 29.096 50.394 1.000 13.03 N SER ANISOU 63 N 1722 1636 1593 -565 -601 4 9 0 ATOM CA SER 22.861 30.224 64 49.718 1.000 12.55 ANISOU 64 CASER 1591 1468 1708 -392 -438 3 1 5 ATOM CB SER 65 23.743 31.472 49.761 1.000 15.41 ANISOU 65 CB SER 2385 1833 1637 -915 -1057 7 8 3 66 OG SER 32.539 23.138 ATOM 49.007 1.000 17.99 ANISOU 66 OG SER. 2.50.4 1721 -718 9.. 2611 -999 9 2 4 C 29.868 ATOM 67 SER 22.520 48.276 1.000 12.72 ANISOU 67 C SER 2040 1187 1606 -576 4 7 6 9 -411 68 0 SER 9 23.397 29.495 ATOM 47.478 1.000 16.18 ANISOU 68 SER 2265 2053 1830 0 9 -465 -3817369 ATOM N LEU 21.229 29.982 47.968 10 1.000 14.19 ANISOU 69 LEU N 10 2154 1488 1750 -301 -699 1 7 4 CALEU ATOM 70 10 20.798 29.714 46.596 1.000 14.62 ANISOU 70 LEU 10 CA2243 1579 -184-784 2 2 4 1734 71 CB LEU 29.883 ATOM 10 19.291 1.000 14.72 46.436 ANISOU 71 LEU 10 2222 1714 CB1657 -142 -657 - 168 ATOM CG LEU 29.633 72 10 18.693 45.050 1.000 14.10 ANISOU 72 LEU 10 CG 2087 1557 1713 -702 -695 1 4 5 73 CD1 LEU ATOM 18.986 28.214 1.000 16.23 10 44.582 ANISOU 73 CD1 LEU 10 -1132 8 7 2994 1578 1595 -554 ATOM CD2 LEU 74 10 17.198 29.913 44.997 1.000 21.82 CD2 LEU ANISOU 74 10 2180 -1151 - 518 2904 3206 -421 LEU 1.000 15.87 C ATOM 75 21.531 30.639 10 45.626 ANISOU 75 C LEU 2449 1785 10 1796 -491 -844314ATOM 76 LEU 10 21.962 30.199 44.553 0 1.000 16.33 ANISOU 76 LEU 2607 1816 -829 2 7 6 0 10 1780 -601 ALA 11 21.669 ATOM 77 31.917 45.986 1.000 17.17 N ANISOU 77 ALA 2521 1889 -548 1 3 9 N 11 2115 -607 1.000 16.56 ATOM 78 CA ALA 11 22.335 32.912 45.129 ANISOU 78 1884 CA ALA 11 2377 2029 -732 -1033 3 0 2 79 ATOM CB ALA 11 22.199 34.259 1.000 20.05 45.805 ANISOU 79 CB ALA 11 3210 1877 -6742592529 -670 MOTA 80 ALA 11 23.786 44.831 1.000 16.33 C 32.535 ANISOU 80  $\mathsf{C}$ 2255 2319 1629 -754 -988 4 3 4 ALA 11 ATOM 81 ALA 24.260 32.587 1.000 19.66 0 11 43.677 ANISOU 81 ALA 11 3115 2559 1795 -947 -560 6 1 9 32.085 45.810 1.000 17.28 ATOM 82 GLU 12 24.558 N ANISOU 82 GLU 12 2686 1994 1884 N -454 -1087 3 9 0 12 GLU 25.931 31.654 45.752 1.000 16.34 ATOM 83 CA ANISOU 83 GLU CA12 2703 1674 1831 -474 -889 1 0 3 3 12 CB GLU 26.527 ATOM 84 31.477 47.158 1.000 16.09 ANISOU 84 CB GLU 12 2440 1867 1808 -770 -820 1 0 5 8 ATOM 85 CG GLU 12 26.633 32.802 47.915 1.000 18.90 ANISOU 85 2335 -1216 -1090 788 CG GLU 12 2717 2127 ATOM 27.115 GLU 12 86 CD 32.657 49.342 1.000 21.17 ANISOU 86 GLU 12 2547 CD 3300 2198 -1182 -1053 7 2 4 ATOM 87 OE1 GLU 12 31.558 27.538 49.756 1.000 22.07 -720 -1365 797 ANISOU 87 OE1 GLU 12 2722 3014 2650 1.000 29.26 ATOM OE2 GLU 12 33.679 88 27.068 50.059 OE2 GLU ANISOU 88 -1279 -1848 476 12 5764 2634 2722 ATOM 89 C GLU 12 25.997 30.402 44.882 1.000 17.16 ANISOU 89 C GLU 12 2044 2319 2158 -624 -715 4 8 1 ATOM 30.317 90 0 GLU 12 26.879 44.032 1.000 18.88 GLU ANISOU 90 12 0 3200 2388 1583 -1004 -306 8 9 9 ATOM 25.083 91 LEU 13 29.441 45.049 1.000 17.32 N ANISOU 91 2176 LEU 13 2300 2104 -659 -386 9 4 N ATOM LEU 92 CA13 25.082 28.252 44.189 1.000 14.00

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ANISOU 92 CA LEU 13 1734 1873 1713 -140 -170 4 9 8 ATOM CB LEU 93 13 24.003 27.248 44.620 1.000 15.37 ANISOU 93 CB LEU 13 2205 1838 1795 -375 -149465ATOM CG 94 LEU 13 24.154 26.554 45.967 1.000 14.52 ANISOU 94 CG LEU 13 1913 1803 1799 -280 -204 4 4 2 CD1 LEU ATOM 95 13 22.934 25.680 46.193 1.000 15.15 ANISOU 95 CD1 LEU 13 2174 1817 1766 -433 185 175 CD2 LEU MOTA 96 25.411 13 25.690 46.067 1.000 17.54 CD2 LEU ANISOU 96 13 2119 2043 2502 -419 2 7 0 -38 MOTA 97 C 24.876 LEU 13 28.626 42.725 1.000 16.54 ANISOU 97 C LEU 13 2510 2062 1710 -222 -93 565 ATOM 98 LEU 0 13 25.548 28.122 41.821 1.000 18.28 ANISOU 98 LEU 0 13 2685 2514 1748 -687 75 2 5 9 ATOM 99 GLN M 23.945 29.534 42.472 1.000 16.86 14 ANISOU 99 1970 N GLN 14 2337 2100 -557 -683 8 3 8 ATOM 100 CAGLN 14 23.657 41.132 1.000 18.63 30.015 ANISOU 100 2761 CAGLN 14 2404 1915 -610 -802 5 6 8 ATOM 101 GLN CB 14 22.421 30.923 41.130 1.000 19.39 ANISOU 101 GLN CB 14 3166 -918 9 7 7 2176 2025 -392 ATOM 102 GLN 21.108 CG14 30.250 41.460 1.000 19.00 ANISOU 102 CG GLN 14 2879 2383 1957 -209 -725 4 6 0 ATOM 103 GLN CD14 19.974 31.227 41.766 1.000 18.83 ANISOU 103 GLN CD14 3139 2118 1897 -6 -1229 4 9 4 OE1 GLN ATOM 104 32.317 14 20.177 42.314 1.000 26.10 ANISOU 104 OE1 GLN 14 3928 2407 3582 -98 -1172 - 241ATOM 105 NE2 GLN 14 18.745 30.823 41.411 1.000 20.94 NE2 GLN ANISOU 105 2716 14 2900 2340 -149 -840 4 5 4 ATOM 106 C GLN 30.812 40.525 1.000 20.40 14. 24.804 ANISOU 106 14 GLN C 3226 2458 2065 -795 -712 9 3 7 107 ATOM 0 GLN 14 24.812 30.951 39.311 1.000 30.48 ANISOU 107 GLN 5089 14 0 4340 2152 -2337 -898 1 2 1 1 ATOM 108 GLN  $\mathbf{N}$ 15 41.329 1.000 20.35 25.734 31.309 ANISOU 108 N GLN 3252 15 2452 2030 -1067 -240 4 9 7 ATOM 109 CAGLN 15 26.909 40.884 1.000 21.88 32.041 ANISOU 109 CAGLN 15 3184 3230 1901 -1152 -299 7 8 8 ATOM 110 CB 27.288 GLN 15 33.100 41.920 1.000 22.20 ANISOU 110  ${\tt GLN}$ CB15 2720 3162 2551 -1131 -770 6 9 1 ATOM 111 CG GLN 15 26.450 34.358 41.954 1.000 25.73 ANISOU 111 4496 CG GLN 15 2545 2735 -821 -233 1 2 6 9 ATOM 112 CD GLN 15 26.325 35.021 43.306 1.000 35.76 GLN ANISOU 112 CD 15 6010 3945 3631 -643 -229 - 135 OE1 GLN 113 ATOM 15 34.884 44.225 1.000 49.13 27.145 ANISOU 113 OE1 GLN 15 8425 5866 4378 -2857 -2197 - 564 114 ATOM NE2 GLN 15 35.812 43.489 1.000 51.85 25.255 ANISOU 114 NE2 GLN 15 7190 5567 62 3066 107 6945 ATOM 115 C GLN 15 28.069 31.079 40.625 1.000 23.93 ANISOU 115 GLN C 3451 15 3513 -990 145 884 2127 ATOM 116 GLN 15 29.177 31.448 40.213 1.000 28.95 ANISOU 116 GLN 15 3535 4619 -899 510 1225 2845 ATOM 117 GLY N 27.828 29.794 40.891 1.000 25.86 16 ANISOU 117 GLY 4089 16 3282 2457 -889 -36 469 ATOM 118 CAGLY 28.812 28.763 40.649 1.000 29.00 16 ANISOU 118 CAGLY 16 4785 3562 2671 -677 765 255 ATOM 119 C GLY 28.546 41.814 1.000 25.45 16 29.741 ANISOU 119 GLY 3427 16 3490 1422 6 7 3 2754 -264 ATOM 120 GLY 30.805 27.955 41.625 1.000 29.63 16 ANISOU 12.0 GLY 16 3925 3267 4068 -66 1997 5 2 3 121 ATOM LEU 28.979 43.015 1.000 22.50 17 29.387 ANISOU 121 LEU 17 3266 2713 2569 -39 923 733 ATOM 122 CALEU 17 30.234 28.727 44.172 1.000 21.73 ANISOU 122 CALEU 17 2299 2931 3025 -282 867 748

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MOTA 123 LEU CB 30.124 17 29.921 45.132 1.000 21.23 ANISOU 123 LEU CB2137 2858 17 3071 -620 669 711 17 ATOM 124 CG LEU 30.354 31.274 44.431 1.000 26.12 ANISOU 124 LEU 17 2708 CG 2965 4253 1342 9 3 1 -889 125 CD1 LEU ATOM 29.962 17 32.444 1.000 29.81 45.305 ANISOU 125 CD1 LEU 2515 17 2924 5885 -396 464 303 CD2 LEU 17 ATOM 126 31.808 31.350 43.974 1.000 32.84 ANISOU 126 2845 CD2 LEU 17 3703 5930 -281 1871 2 1 1 4 127 LEU 17 C ATOM 29.886 27.456 1.000 19.36 44.936 ANISOU 127 LEU 2819 C 17 2.0.81 2455 -239 545 580 ATOM 128 LEU 26.920 0 17 28.773 44.848 1.000 21.11 ANISOU 128 LEU 0 17 2284 3004 2734 -444 107 1055 129 N 18 ATOM HIS 30.838 26.952 45.706 1.000 21.02 ANISOU 129 18 Ν HIS 2124 2752 3109 -314 193 4 9 1 ATOM HIS 130 CA 18 30.678 46.615 25.814 1.000 18.11 ANISOU 130 HIS 18 CA1569 2996 2315 -460 -28 3 6 1 131 CB HIS 18 26.149 47.702 MOTA 29.655 1.000 21.25 ANISOU 131 HIS CB1731 18 3332 3010 -45 282 3 5 4 132 29.796 ATOM CG HIS 18 27.515 48.283 1.000 23.28 ANISOU 132 CG HIS 18 2234 3612 2999 211 -46 - 20133 ATOM CD2 HIS 18 28.898 1.000 24.53 28.535 48.344 CD2 HIS ANISOU 133 41 4 4 0 18 3112 3479 2728 532 ATOM 134 ND1 HIS 18 30.940 27.977 48.895 1.000 26.72 ANISOU 134 ND1 HIS 18 2938 4039 3173 -151 -569 3 8 CE1 HIS ATOM 135 18 30.756 29.218 49.307 1.000 29.80 ANISOU 135 CE1 HIS 18 4476 3775 3071 -542 -562 2 3 7 NE2 HIS ATOM 136 18 29.524 29.581 48.985 1.000 30.03 ANISOU 136 NE2 HIS 18 :4752 3282 3377 216 -148 3 3 8 137 C HIS ATOM 18 30.266 24.528 45.917 1.000 18.57 ANISOU 137 HIS C 18 1943 30 5 9 0 3084 2028 -951 ATOM 138 18 0 HIS 29.594 46.532 23.682 1.000 19.92 ANISOU 138 HIS 18 0 1949 3125 2493 -777 -87 995 ATOM 139 N 19 30.647 GLN 24.340 44.658 1.000 19.24 ANISOU 139 19 2329 N GLN 2700 2282 -256 298 CA ATOM 140 19 30.119 43.908 GLN 23.206 1.000 21.51 ANISOU 140 CA GLN 3249 19 2431 . 2492 597 -228 3 1 8 ATOM 30.446 141 GLN CB 19 1.000 22.89 23.307 42.406 ANISOU 141 GLN 3231 CB 3058 2408 19 -148 463 2 4 4 ATOM 142 CG GLN 29.738 19 24.453 41.698 1.000 25.83 ANISOU 142 CG GLN 19 3445 3712 2658 -407 5 6 8 -384 143 ATOM CD GLN 19 28.223 24.470 41.747 1.000 31.56 ANISOU 143 CD GLN 3832 19 3439 4722 -252 -988 3 5 7 OE1 GLN 23.640 ATOM 144 19 27.521 41.153 1.000 38.51 ANISOU 144 OE1 GLN 19 3869 3649 7115 377 -3045 686 NE2 GLN MOTA 145 19 27.621 25.433 42.475 1.000 33.32 ANISOU 145 NE2 GLN 5695 19 3303 3663 647 -1109 449 146 GLN ATOM 19 C 30.578 21.873 44.485 1.000 20.32 ANISOU 146 C GLN 19 2224 514 3 9 4 2710 2785 -60 ATOM 147 GLN 19 29.806 0 20.900 44.473 1.000 19.08 ANISOU 147 GLN 0 2451 2910 221 257 743 19 1888 ATOM 148 ASP 31.800 21.761 44.999 1.000 24.09 20 N ANISOU 148 ASP 2645 20 3001 3507 -773 -507 4 1 5 N ATOM 149 ASP 20 CA32.268 45.553 1.000 21.82 20.498 ANISOU 149 ASP CA 1707 3811 2774 -327 -58 357 20 150 MOTA ASP CB 33.780 20.527 45.779 1.000 26.34 20 ANISOU 150 ASP -962 236 490 CB 20 1594 4552 3863 ATOM 151 CG ASP 20.517 34.596 20 44.503 1.000 34.45 ANISOU 151 CG ASP 5859 2531 20 4701 -1208 1213 - 280 ATOM 152 19.982 43.457 1.000 33.11 OD1 ASP 34.177 20 OD1 ASP ANISOU 152 20 3768 4173 4640 -311 1233 - 375 ATOM 153 OD2 ASP 35.725 20 21.056 44.532 1.000 49.71

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OD2 ASP
 ANISOU 153
                      20
                           3445
                                   9922
                                           5519
                                                   -3116 1710 5 3
MOTA
        154
             C
                 ASP
                      20
                           31.538
                                   20.179 46.862 1.000 21.03
ANISOU 154
             \mathsf{C}
                 ASP
                      20
                           1876
                                   2702
                                           3412
                                                   -231 616 388
ATOM
        155
                 ASP
             0
                      20
                           31.118
                                           47.075 1.000 20.80
                                   19.038
ANISOU 155
             0
                 ASP
                      20
                           1162
                                   2583
                                           4157
                                                   -72
                                                         -139 5 5 0
ATOM
        156
                           31.359
             N
                 GLU
                      21
                                   21.177
                                           47.729 1.000 17.88
ANISOU 156
             N
                 GLU
                      21
                          1218
                                   2751
                                           2824
                                                   -263
                                                         -148 5 1 1
ATOM
       157
             CY
                 GLU
                      21
                          30.599
                                   20.999
                                           48.965 1.000 16.80
ANISOU 157
             CA
                          1128
                 GLU
                      21
                                   2173
                                           3083
                                                   -96
                                                         46 3 9 4
ATOM
       158
                          30.654
             CB
                      21
                 GLU
                                   22.304
                                           49.781 1.000 20.23
ANISOU 158
             CB
                 GLU
                      21
                          1366
                                   2620
                                           3701
                                                   5 -262 -210
ATOM
       159
             CG
                 GLU
                      21
                          32.040
                                   22.669
                                           50.307 1.000 24.60
ANISOU 159
                          1660
             CG
                 GLU
                      21
                                   3325
                                           4359
                                                   -221 -654 - 301
MOTA
       160
             CD
                 GLU
                      21
                          32.860
                                           49.402 1.000 28.46
                                   23.565
ANISOU 160
             CD
                 GLU
                      21
                          1191
                                   4348
                                           5275
                                                   -498 -1597 1125
       161
             OE1 GLU
ATOM
                          33.751
                      21
                                   24.294
                                           49.919 1.000 31.17
ANISOU 161
             OE1 GLU
                          2360
                      21
                                   4428
                                           5057
                                                   -1039 -1094 3 4 9
ATOM
       162
             OE2 GLU
                          32.664
                      21
                                   23.590
                                           48.171 1.000 31.16
             OE2 GLU
ANISOU 162
                      21
                          2734
                                                   -1519 -1565 1123
                                   3901
                                           5203
ATOM
       163
             C
                 GLU
                      21
                          29.159
                                           48.689 1.000 16.44
                                   20.594
ANISOU 163
             \mathsf{C}
                 GLU
                      21
                                   2295
                          1271
                                           2679
                                                   -165 -53 430
ATOM
       164
             0
                 GLU
                      21
                          28.599
                                   19.700
                                           49.329 1.000 14.30
ANISOU 164
             0
                 GLU
                      21
                          1271
                                   2257
                                           1907
                                                   -417 -301 3 6
ATOM
       165
                 PHE
             N
                      22
                                   21.257
                          28.548
                                           47.708 1.000 16.14
ANISOU 165
             N
                 PHE
                      22
                          1440
                                   2441
                                           2253
                                                   -316 -28 328
ATOM
       166
             CA
                 PHE
                      22
                                   20.947
                          27.155
                                           47.327
                                                   1.000 15.36
ANISOU 166
             CA
                 PHE
                      22
                          1530
                                   2012
                                           2294
                                                   -262 -173 2 8 1
ATOM
       167
             CB
                 PHE
                      22 _ 26.612
                                   21.967
                                           46.343
                                                   1.000 15.43
ANISOU 167
             CB
                 PHE
                      22
                                   2056
                          1863
                                           1944
                                                   -316 -247 1 8 4
ATOM
       168
             CG
                 PHE
                      22
                          25.119
                                   21.932
                                           46.077
                                                   1.000 15.59
ANISOU 168
             CG
                 PHE
                      22
                                   2141
                          1822
                                           1962
                                                   -299 -170 5 6 1
            CD1 PHE
MOTA
       169
                      22
                          24.218
                                   21.987
                                           47.129
                                                  1.000 17.03
ANISOU 169
            CD1 PHE
                      22
                                   2605
                          1923
                                           1943
                                                   -410 -162 - 40
            CD2 PHE
ATOM
       170
                          24.606
                      22
                                   21.856
                                           44.797 1.000 14.84
ANISOU 170
            CD2 PHE
                          1541
                      22
                                   2083
                                                   51 -94 - 155
                                           2013
ATOM
            CE1 PHE
       171
                      22
                          22.861
                                  21.938
                                           46.906
                                                  1.000 15.96
ANISOU 171
            CE1 PHE
                      22
                          1844
                                   1805
                                                   -159 -64 176
                                           2414
ATOM
       172
            CE2 PHE
                          23.243
                      22
                                   21.797
                                           44.551 1.000 15.81
ANISOU 172
            CE2 PHE
                      22
                          1600
                                   1993
                                           2416
                                                   -261 -190 - 176
ATOM
       173
            CZ
                 PHE
                      22
                          22.360
                                   21.853 45.612 1.000 14.18
ANISOU 173
            CZ
                 PHE
                      22
                          1427
                                   1430
                                        2531 -105 -164 3 2 5
ATOM
       174
                 PHE
            C
                     22
                          27.049
                                  19.515 46.792 1.000 16.23
ANISOU 174
            C
                 PHE
                          1325
                      22
                                   2042
                                           2797
                                                  -110 164 102
ATOM
       175
                 PHE
                      22
                          26.183
                                  18.751 47.229 1.000 13.24
ANISOU 175
                 PHE
            0
                      22
                          1411
                                   1743
                                           1876
                                                   105
                                                         -194 3 9 1
ATOM
       176
                 ARG
                          27.888
                      23
                                  19.097 45.853 1.000 15.45
ANISOU 176
                 ARG
                      23
                          1585
                                   2313
                                           1971
                                                   -167 -80 289
ATOM
       177
            CA
                          27.865 17.746 45.325 1.000 15.49
                 ARG
                      23
ANISOU 177
            CA
                ARG
                          809 2443
                     23
                                       2634
                                               50 -41 - 22
ATOM
       178
            CB
                ARG
                      23
                          28.928 17.539 44.248 1.000 17.81
ANISOU 178
            CB
                ARG
                     23
                          966 3142
                                       2658
                                               -128 43 - 167
ATOM
       179
            CG
                ARG
                          28.470 17.928 42.860 1.000 25.86
                      23
ANISOU 179
            CG
                      23
                 ARG
                          2719
                                   4636
                                           2470
                                                   -758 -176 - 4 9
ATOM
       180
            CD
                 ARG
                      23
                          29.485
                                  17.370 41.867 1.000 34.68
ANISOU 180
            CD
                ARG
                      23
                          5148
                                           3183
                                   4847
                                                   -1532 1634 - 548
ATOM
       181
            ΝE
                ARG
                      23
                          30.660
                                  18.253 41.877 1.000 31.13
ANISOU 181
            NΞ
                 ARG
                      23
                          2799
                                   4194
                                           4836
                                                         747 6 6
                                                   305
ATOM
       182
                ARG
            CZ
                      23
                                  19.424 41.244 1.000 34.24
                          30.703
ANISOU 182
            CZ
                ARG
                      23
                          2749
                                   4844
                                           5418
                                                   -757 239 764
ATOM
       183
            NH1 ARG 23
                          29.647
                                  19.856 40.551 1.000 28.06
ANISOU 183
            NH1 ARG
                     23
                          2714
                                   3685
                                           4263
                                                   -721 555 181
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ATOM 184 NH2 ARG 23 31.830 20.114 41.340 1.000 36.08 ANISOU 184 NH2 ARG 23 2261 5328 6121 -562 776 - 86 ATOM 185 C ARG 23 28.045 16.713 46.420 1.000 15.06 ANISOU 185 C ARG 23 1071 2589 167 -32 - 2342061 186 23 27.335 MOTA ARG 0 15.687 46.410 1.000 16.28 ANISOU 186 ARG 23 0 1443 2244 2497 -118 -71 - 277ATOM 187 24 Ν ARG 28.952 16.988 47.353 1.000 15.27 ANISOU 187 ARG N 2623 24 2156 1024 -52 -21 2 9 188 24 ATOM CAARG 29.193 16.003 48.430 1.000 17.70 ANISOU 188 ARG 24 CA2589 2693 1443 275 -2 2 1 5 189 CB ARG 24 ATOM 30.466 16.422 49.148 1.000 21.11 ANISOU 189 CB ARG 24 1244 3289 3486 484 -257 3 8 4 31.787 190 CG ARG ATOM 24 16.217 1.000 30.46 48.429 ANISOU 190 ARG CG 1438 5078 24 5057 426 441 3 0 8 191 CD ARG ATOM 24 32.979 16.537 49.330 1.000 33.50 ANISOU 191 CD ARG 24 1163 5831 5736 208 370 458 192 ARG 33.636 ATOM NE 24 17.804 49.071 1.000 51.46 ANISOU 192 24 NE ARG 5800 7316 6437 -2596 -1688 1165 ATOM 193 CZARG 24 18.776 49.903 1.000 46.72 33.973 ANISOU 193 CZARG 24 4738 6888 6124 -1719 -1822 1316 NH1 ARG ATOM 194 24 33.731 51.213 1.000 44.24 18.728 ANISOU 194 NH1 ARG 24 2650 6998 7160 -392 1001 8 4 NH2 ARG ATOM 195 24 34.579 19.871 49.448 1.000 42.82 NH2 ARG ANISOU 195 24 5339 6503 -991 1216 4428 513 15.887 49.334 1.000 17.16 ATOM 196 C ARG 24 27.972 ANISOU 196 C ARG 24 1549 2071 2900 129 140 2 9 5 197 ATOM 0 ARG 24 27.536 14.779 49.713 1.000 15.38 24 = 1706 ANISOU 197 ARG 0 1890 2247 72 - 388CYS 25 ATOM 198 N 27.355 17.011 49.696 1.000 12.91 ANISOU 198 CYS 25 N 907 1824 2176 -254 - 386CYS ATOM 199 CA25 26.105 17.040 50.454 1.000 12.45 ANISOU 199 CYS CA25 942 1838 1949 -178 - 480 8 1ATOM 200 CYS CB 25 25.660 18.491 50.697 1.000 11.67 ANISOU 200 CYS 25 CB 1150 1759 1527 -136 -604 1 8 4 23.973 ATOM 201 CYS SG 25 18.580 51.425 1.000 14.90 ANISOU 201 CYS 25 SG 1593 2602 -164 - 26 - 181465 ATOM 16.225 49.769 1.000 11.67 202 CYS 25 25.001 C C -283 -64 -86 ANISOU 202 CYS 25 893 1897 1645 24.360 15.377 50.390 1.000 12.73 ATOM 203 CYS 25 0 ANISOU 203 CYS 0 25 1347 2064 1426 -233 -196 1 2 3 204 · N ATOM 24.798 16.461 48.470 1.000 11.70 LEU 26 ANISOU 204 LEU N 1102 26 1530 1814 -128 -3901ATOM 205 LEU CA26 23.766 47.735 1.000 11.11 15.716 ANISOU 205 LEU CA1190 26 1476 1556 -238 -79 -194ATOM 206 CB 26 16.198 46.285 1.000 11.54 LEU 23.674 ANISOU 206 1345 CBLEU 1522 1518 -75 -84 - 20226 MOTA 207 CG LEU 26 23.242 17.638 46.019 1.000 12.42 ANISOU 207 CG LEU 26 1199 1542 1978 -153 - 167 - 40MOTA 208 CD1 LEU 26 23.414 17.993 44.539 1.000 14.77 ANISOU 208 CD1 LEU 43 131 4 0 1 1428 1916 2270 26 ATOM 209 CD2 LEU 46.466 1.000 14.45 21.814 26 17.885 ANISOU 209 CD2 LEU 26 1384 264 -32 3 2 1 2061 2047 ATOM 210 1.000 12.93 LEU 23.979 C 26 14.209 47.780 -121 -486 - 107 ANISOU 210 C LEU 26 1360 1542 2011 ATOM LEU 48.008 1.000 13.78 211 26 0 23.011 13.461 ANISOU 211 LEU 26 -305 -426 - 51 0 1660 1450 2125 ATOM 212 ARG N 25.196 27 13.721 47.576 1.000 14.09 ANISOU 212 ARG 1518 N27 1729 151 -530 - 1052108 MOTA 213 CAARG 27 12.283 25.491 47.574 1.000 15.39 ANISOU 213 CA27 ARG 1690 1897 2260 186 141 - 354ATOM 214 CBARG 27 26.846 12.122 46.900 1.000 17.04

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ANISOU 214 CB ARG2259 27 2356 1861 517 49 - 248 MOTA 215 CG ARG 27 27.502 10.780 46.801 1.000 25.08 ANISOU 215 CG ARG 27 2837 3110 3583 1105 606 - 399 ATOM 216 ARG 27 28.995 CD 10.992 46.457 1.000 30.32 ANISOU 216 CD ARG 27 2976 3836 1190 720 -1381 4710 ATOM 217 ARG 27 NΞ 29.818 11.407 47.581 1.000 36.51 ANISOU 217 3633  $N\Xi$ ARG 27 4937 5301 391 -1429 121 12.019 ATOM 218 CZARG 27 30.988 1.000 38.07 47.560 ANISOU 218 CZ27 ARG 3334 5192 5941 364 661 - 1776 219 ATOM NH1 ARG 27 31.565 46.401 12.340 1.000 48.56 ANISOU 219 27 .7688 NH1 ARG 4482 6280 -1305 736 -1326 220 ATOM NH2 ARG 27 12.328 31.606 48.701 1.000 40.23 ANISOU 220 NH2 ARG 27 2891 6127 6266 457 717 -2463 221 C ATOM ARG 27 25.479 11.630 1.000 14.66 48.949 ANISOU 221 C ARG 27 1720 1617 2233 135 -33 - 42222 ATOM 0 ARG 27 24.968 10.499 49.072 1.000 17.44 ANISOU 222 0 ARG 27 1981 1533 3114 98 - 394155 ATOM 223 28 49.973 1.000 13.72 Ν ASP 26.031 12.308 ANISOU 223 N ASP 28 1703 1366 2146 317 -327319224 26.227 ATOM CAASP 28 51.277 1.000 15.33 11.701 ANISOU 224 CAASP 28 1886 1704 2234 538 -247391225 CB. ATOM ASP 28 12.280 1.000 18.31 27.541 51.842 ANISOU 225 2092 CB ASP 28 2709 2155 186 -465 5 4 4 226 ASP ATOM CG 28 ,28.785 11.875 1.000 23.06 51.083 ANISOU 226 CG ASP 28 2002 3583 3176 -96 -50 478 ATOM 227 OD1 ASP 28 28.741 10.904 1.000 25.09 50.290 ANISOU 227 OD1 ASP 28 2515 2855 4163 830 406 440 OD2 ASP 28 228 ATOM 12.528 29.831 51.283 1.000 30.05 ANISOU 228 OD2 ASP 5236 28 1919 4262 -695 1 0 5 8 -216 229 25.092 MOTA C ASP 28 11.910 52.267 1.000 14.90 1435 ANISOU 229 C ASP 28 2071 2154 -203217411 230 ATOM ASP 0 28 24.967 11.093 53.200 1.000 14.50 ANISOU 230 ASP 0 28 1878 1501 2132 444 -265 1 7 9 231 ATOM Ν LYS 29 24.317 12.975 52.096 1.000 12.90 ANISOU 231 LYS 29 1290 N1487 2126 77 - 2761 3 6 MOTA 232 CALYS 23.265 13.368 53.029 1.000 12.95 29 ANISOU 232 CA29 LYS 1369 1649 1904 8 -390 MOTA 233 CB 29 LYS 23.699 14.653 53.763 1.000 12.71 ANISOU 233 LYS CB 29 1105 1581 -359 - 302145 209 MOTA CG 234 LYS 29 25.016 14.504 54.518 1.000 16.11 ANISOU 234 CG LYS 29 2711 . 1998 1413 21 -818 LYS ATOM 235 15.727 55.309 1.000 18.24 29 CD 25.449 ANISOU 235 2500 CDLYS 29 1989 2442 -47 -1140 - 14ATOM 236 LYS CE 29 26.789 15.445 56.002 1.000 19.36 ANISOU 236 CE LYS 2148 29 2038 3171 -822 - 725-90 ATOM 237 NZLYS 27.515 29 16.696 56.351 1.000 26.61 ANISOU 237 29 NZLYS 2592 3146 4373 -309 -1571 -353 238 ATOM C LYS 29 13.550 52.386 1.000 11.62 21.888 ANISOU 238 LYS C 29 1432 1831 1153 52 - 290 2 4 239 ATOM 20.877 13.028 0 LYS 29 52.880 1.000 12.57 ANISOU 239 LYS 1426 0 29 1556 1792 -97 -282 1 0 0 ATOM 240 N GLY 21.779 14.280 51.284 1.000 11.98 30 ANISOU 240 GLY 30 N 1359 1454 1741 -5 -310 7 8 ATOM 241 GLY CA30 20.510 14.478 50.562 1.000 10.93 ANISOU 241 CA30 1192 GLY -158 -116 - 18 1497 1465 242 ATOM GLY C 19.544 15.433 51.242 1.000 11.15 30 ANISOU 242 C GLY 30 1137 1143 1955 -260 - 154 - 131ATOM 243 GLY 15.374 50.963 1.000 11.26 30 18.337 ANISOU 243 GLY 30 1247 1082 1949 -56 -419 1 0 4 ATOM 244 LEU N 31 20.064 16.278 52.129 1.000 10.54 ANISOU 244 N LEU 31 1292 894 1821 -98 -367 8 9

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CA17.324 52.803 MOTA 245 19.272 LEU 31 1.000 11.07 CALEU 31 ANISOU 245 1345 1111 1752 46 - 520 - 33 ATOM 246 31 CB LEU 18.465 16.777 53.975 1.000 14.44 2062 ANISOU 246 31 1753 CB LEU 1671 -284 - 80 - 178MOTA 247 31 19.113 CG LEU 16.629 55.333 1.000 17.74 ANISOU 247 LEU CG 2456 31 2220 2064 -172 -115 4 9 9 15.978 56.371 CD1 LEU ATOM 248 18.220 31 1.000 26.19 ANISOU 248 CD1 LEU 2716 31 4691 2543 -1224 -213 1 0 1 6 249 CD2 LEU 15.821 55.182 31 20.388 ATOM 1.000 22.77 ANISOU 249 CD2 LEU 31 3121 2899 2633 650 -18 1487 250 LEU 31 ATOM  $\mathsf{C}$ 20.176 18.498 53.195 1.000 10.95 ANISOU 250 1129 31 C LEU 1041 180 1989 -318 - 223ATOM 251 18.314 53.424 0 LEU 21.376 31 1.000 10.89 ANISOU 251 LEU 0 1015 31 1171 1952 69 - 160 204 252 PHE ATOM N19.570 32 19.688 53.219 1.000 11.42 ANISOU 252 PHE 32 1134 N 995 2211 75 -273 6 5 ATOM 253 32 20,280 20.916 53.545 1.000 10.33 CAPHE ANISOU 253 CA32 PHE 1071 1703 -57 1152 -288 - 33254 PHE ATOM CB 32 21.307 52.422 1.000 12.25 21.244 ANISOU 254 CB PHE 1054 32 1729 1872 -113 -173 - 5ATOM 255 32 CG PHE 20.624 51.041 1.000 11.94 21.346 ANISOU 255 CG PHE 32 -148 1 2 2 1158 1572 -281 1809 256 ATOM CD1 PHE 32 20.522 20.188 50.270 1.000 11.12 ANISOU 256 CD1 PHE 1308 1070 32 1846 -182 -458 3 1 8 257 ATOM CD2 PHE 32 20.145 22.528 50.513 1.000 12.14 ANISOU 257 CD2 PHE 32 1618 1353 1639 -300 -185 - 47258 CE1 PHE 32 ATOM 19.943 20.212 49.015 1.000 12.00 ANISOU 258 CE1 PHE 32 \_1342 1377 1840 -301 -468 3 3 2 259 22.534 49.266 1.000 12.79 CE2 PHE ATOM 32 19.553 ANISOU 259 CE2 PHE 32 1858 1543 1457 -86 -34 2 8 260 21.376 ATOM CZPHE 32 19.416 48.503 1.000 11.50 ANISOU 260 PHE CZ32 1623 1414 1331 -76 -272 2 1 7 ATOM 261 C PHE 32 19.310 22.071 53.762 1.000 9 . 8 2 C ANISOU 261 PHE 32 1015 1042 1674 -120 -367 - 77262 ATOM 18.165 Q 32 21.990 53.285 PHE 1.000 11.29 ANISOU 262 PHE 32 1097 0 1286 1906 -95 -495 - 77ATOM 263 TYR 33 19.736 N 23.099 54.493 1.000 12.68 ANISOU 263 N 33 1606 1053 -766 - 159 TYR -57 2158 ATOM 264 24.335 54.607 1.000 10.64 CATYR 18.945 33 ANISOU 264 CA1491 TYR 33 1173 1380 -77 -97 - 132TYR 33 19.141 25.022 55.955 1.000 10.85 ATOM 265 CB ANISOU 265 CB TYR 33 1019 1725 1379 -260 -224 - 164 ATOM 266 CG TYR 33 18.545 24.331 57.156 1.000 10.71 ANISOU 266 1342 CG TYR 33 1173 1552 -230 - 117-45 267 17.266 24.643 57.619 1.000 11.64 MOTA CD1 TYR 33 CD1 TYR ANISOU 267 1441 33 1385 1596 -68 83 - 94 MOTA 268 CE1 TYR 16.694 24.023 58.719 1.000 13.60 33 CE1 TYR 33 ANISOU 268 1804 1879 1483  $-147 \cdot 339 - 26$ ATOM 269 CD2 TYR 19.273 23.364 57.853 1.000 14.04 33 CD2 TYR 33 ANISOU 269 1604 2040 1689 132 -509 1 2 7 ATOM 270 CE2 TYR 33 18.711 22.752 58.964 1.000 15.75 ANISOU 270 CE2 TYR 33 1872 2227 1886 -187 -701433ATOM 33 17.438 23.078 59.387 1.000 16.02 271 ÇΖ TYR ANISOU 271 CZ2205 TYR 33 1939 -332 -154 3 0 0 1942 ATOM 272 OH TYR 33 16.919 22.454 60.504 1.000 19.95 ANISOU 272 -60 278 400 TYR OH33 3412 2154 2015 MOTA 273 C TYR 33 19.357 25.253 53.452 1.000 10.92 ANISOU 273 33 1249 TYR C 1448 1453 -125 -271 1 4 9 ATOM 274 TYR 33 20.514 25.192 53.006 1.000 11.50 0 ANISOU 274 TYR 33 1204 Q 1375 1791 -98 -270 2 8 1 275 ATOM LEU N 34 18.399 26.049 53.000 1.000 11.28

- 99 -ANISOU 275 LEU 34 1159 1265 -210 -149 1 2 1 1862 276 MOTA CALEU 34 18.577 26.942 51.864 1.000 12.99 ANISOU 276 CALEU 34 1565 1926 1444 81 - 4782 7 4 277 ATOM CBLEU 34 17.757 50.682 1.000 13.96 26.420 ANISOU 277 CB LEU 34 2007 1301 1995 -430 -459 3 2 1 278 MOTA CG LEU 34 17.990 27.112 49.334 1.000 13.81 ANISOU 278 CG LEU 1322 34 2085 1839 -331 -365 1 9 8 279 ATOM CD1 LEU 34 19.308 48.704 1.000 15.94 26.691 ANISOU 279 CD1 LEU 34 2123 1793 2140 -10 -313 6 0 7 280 ATOM CD2 LEU 16.818 34 26.799 48.411 1.000 16.36 CD2 LEU ANISOU 280 2186 34 1837 2193 122 -721134281 ATOM C LEU 34 52.241 1.000 13.03 18.195 28.361 ANISOU 281 LEU C 1676 34 1418 1857 31 - 6432 1 8 ATOM 282 0 LEU 34 17.055 52.595 1.000 13.99 28.647 ANISOU 282 0 LEU 1690 34 1281 2344 140 -714 8 5 ATOM 283 N35 THR 19.148 29.283 52.175 1.000 15.03 ANISOU 283 N THR 35 1837 1584 2288 -118 -625 - 3ATOM 284 CATHR 3 5 18.918 30.704 52.369 1.000 14.80 ANISOU 284 CATHR 35 1866 1560 2196 -169 -175 - 144 ATOM 285 THR CB35 20.013 53.232 1.000 15.65 31.366 ANISOU 285 CBTHR 35 2025 1719 2202 -149 -204 - 281286 ATOM OG1 THR 35 21.276 31.115 52.601 1.000 18.81 OG1 THR ANISOU 286 3 5 1885 2679 2583 -279 -229 - 728CG2 THR 287 ATOM 35 20.138 30.811 54.622 1.000 18.84 ANISOU 287 CG2 THR 35 2523 2207 2427 -850 -510 1 5 5 288 MOTA C THR 35 18.915 51.043 1.000 15.07 31.456 ANISOU 288 C THR 35 1904 1473 2348 -57 -283 - 70289 ATOM THR 0 35 30.909 49.973 1.000 15.00 19.209 ANISOU 289 35 <sup>2</sup> 2034 THR 0 1520 2145 -215 -372 8 9 ATOM 290 N ASP 36 18.564 32.739 51.086 1.000 17.46 ANISOU 290  $\mathbf{N}$ ASP 36 2302 1366 2968 -209 -766 - 12.0ATOM 291 CAASP 36 18.618 33.606 49.924 1.000 17.91 ANISOU 291 ASP CA 36 2150 1592 3063 -660 8 6 112 ATOM 292 CB ASP 36 20.063 33.845 49.471 1.000 17.91 ANISOU 292 CBASP 2153 36 1584 3067 84 -587 - 4 2 293 ATOM CG ASP 20.948 36 34.545 50.469 1.000 19.23 ANISOU 293 CG ASP 36 2575 2160 2571 -642 -324 1 8 1 294 OD1 ASP ATOM 36 20.426 35.304 51.325 1.000 24.17 ANISOU 294 OD1 ASP 3055 36 2843 3284 152 -1013 - 652295 ATOM OD2 ASP 22.199 36 34.355 50.412 1.000 21.00 ANISOU 295 OD2 ASP 36 2637 2571 2772 -382 -834 - 393ATOM 296 36 48.784 1.000 18.20 ASP 33.038 17.783 ANISOU 296 C ASP 2402 36 1736 2779 -446 -390 1 9 1 297 ATOM ASP 36 18.222 47.629 1.000 18.98 33.063 ANISOU 297 ASP 36 2127 2022 3062 -464 -60 -252 ATOM 298 N CYS 37 16.593 32.547 49.077 1.000 17.22 ANISOU 298 N CYS 37 1873 2190 2479 63 - 350 - 1ATOM 299 CACYS 37 15.730 31.945 48.043 1.000 15.98 ANISOU 299 CYS CA1997 37 1590 2485 -65 -184 -81 ATOM 300 CYS CB37 48.252 1.000 18.87 15.621 30.423 ANISOU 300 CYS CB 37 2112 1790 3268 -114 -405 5 7 0 ATOM 301 SG CYS 29.917 37 14.753 49.759 1.000 19.42 ANISOU 301 CYS SG 2532 37 1683 3164 -74 -230 3 2 2 ATOM 302 C CYS 14.349 32.580 37 47.958 1.000 16.12 ANISOU 302 C CYS 1992 37 1669 -175 -504 1 6 2465 303 ATOM 0 CYS 13.483 37 32.032 47.253 1.000 20.60 ANISOU 303 CYS 37 2761 1769 3296 -1333 5 1 -241 MOTA 304 N GLY 38 33.714 48.617 1.000 17.89 14.125 ANISOU 304 GLY N 38 1847 1572 3381 209 -898 - 111ATOM 305 GLY CA12.850 34.404 48.587 1.000 18.16 38 ANISOU 305 CA GLY

2126

3164

141

-999 - 6

1608

38

		400		1 6 1/4 1/5 1/5 1/5 1/5 1/5 1/5 1/5 1/5 1/5 1/5
ATOM 306 ANISOU 307 ATOM 308 ATOM 309 ANISOU 309 ANISOU 310 ATOM 311 ANISOU 311 ANISOU 311 ANISOU 311 ATOM 312 ANISOU 313 ATOM 313 ATOM 314 ANISOU 315 ANISOU 315 ANISOU 315 ANISOU 316 ANISOU 317 ANISOU 317 ANISOU 317 ANISOU 317 ANISOU 318 ATOM 318 ANISOU 318 ATOM 321 ANISOU 321 ANISOU 321 ANISOU 322 ANISOU 322 ANISOU 322 ANISOU 322 ANISOU 323 ANISOU 323 ANISOU 323 ANISOU 323 ANISOU 325 ANISOU 325 ANISOU 326 ANISOU 327 ANISOU 327 ANISOU 327 ANISOU 327 ANISOU 328 ANISOU 328 ANISOU 328 ANISOU 329 ANISOU 329 ANISOU 329 ANISOU 329 ANISOU 329 ANISOU 329 ANISOU 3331 ANISOU 3333	Y 38 38 38 39 39 39 39 39 39 39 39 39 39 39 39 39	2598	34930       34930 <td< td=""><td>1.000 21.98 262 -97 -455 1.000 22.75 241 79 -97 1.000 21.93 -65 -102 -154 1.000 26.16 -1071 162 -400 1.000 28.13 -352 -848 258 1.000 27.39 541 -637 -1052 1.000 28.66 581 -150 -190 1.000 30.62 1275 -1485 -208 1.000 26.26 -796 170 335 1.000 26.61 -703 -191 1 0 2 1.000 26.61 -703 -191 1 0 2 1.000 27.03 -690 -220 - 3 1.000 27.03 -690 -220 - 3 1.000 25.98 -546 36 -720 1.000 27.16 -932 -391 1 48 1.000 27.16 -932 -391 1 48 1.000 36.24 -472 -136660 1.000 34.29 -1303 2206429 1.000 28.20 -711 -317 - 479 1.000 28.20 -711 -317 - 479 1.000 28.20 -711 -317 - 479 1.000 28.20 -711 -317 - 479 1.000 28.21 892 -594 -555 1.000 42.46 -1196 -1257 8 26 1.000 55.96 -2654 -82 1 2 4 9 1.000 55.96 -2654 -82 1 2 4 9 1.000 61.55 -4396 -4720 2 3 0 9 1.000 29.30 -1404 -1089 - 72 1.000 33.69 -1524 -819 - 1 2 7 1.000 36.90</td></td<>	1.000 21.98 262 -97 -455 1.000 22.75 241 79 -97 1.000 21.93 -65 -102 -154 1.000 26.16 -1071 162 -400 1.000 28.13 -352 -848 258 1.000 27.39 541 -637 -1052 1.000 28.66 581 -150 -190 1.000 30.62 1275 -1485 -208 1.000 26.26 -796 170 335 1.000 26.61 -703 -191 1 0 2 1.000 26.61 -703 -191 1 0 2 1.000 27.03 -690 -220 - 3 1.000 27.03 -690 -220 - 3 1.000 25.98 -546 36 -720 1.000 27.16 -932 -391 1 48 1.000 27.16 -932 -391 1 48 1.000 36.24 -472 -136660 1.000 34.29 -1303 2206429 1.000 28.20 -711 -317 - 479 1.000 28.20 -711 -317 - 479 1.000 28.20 -711 -317 - 479 1.000 28.20 -711 -317 - 479 1.000 28.21 892 -594 -555 1.000 42.46 -1196 -1257 8 26 1.000 55.96 -2654 -82 1 2 4 9 1.000 55.96 -2654 -82 1 2 4 9 1.000 61.55 -4396 -4720 2 3 0 9 1.000 29.30 -1404 -1089 - 72 1.000 33.69 -1524 -819 - 1 2 7 1.000 36.90
	_	3354 3051 6.026 36.969 3578 2980 9.282 37.967 5831 4318	4667 55.844 7462 56.281 5354	204 -648 - 277
			51.203	1.000 40.30

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		- 101 -		
ANISOU 336	OG1 THR 42	6998 3682	6912	3163 1170 177
ATOM 337	CG2 THR 42	3002		-3163 -1478 1 7 7
ANISOU 337	CG2 THR 42		55.872	1.000 45.59
ATOM 338	N GLU 43		4363	-2166 -1048 2 3 8
ANISOU 338			54.862	1.000 31.74
ATOM 339		3380 4360	4319	-673 -223 - 782
ANISOU 339		6.647 35.355	53.810	1.000 35.40
	CA GLU 43	4856 4683	3913	-1510 -860 3 2 9
ATOM 340	C GLU 43	5.643 34.324	54.330	1.000 28.03
ANISOU 340	C GLU 43	2988 3297	4363	-41 -919 1 6 8
ATOM 341	O GLU 43	4.560 34.138	53.764	1.000 38.18
ANISOU 341	O GLU 43	3818 2970	7717	-66 -2774 1469
ATOM 342	CB GLU 43	7.423 34.811	52.608	1.000 38.89
ANISOU 342	CB GLU 43	4464 6532	3779	-2546 -860 - 393
ATOM 343	CG GLU 43	8.462 35.745	52.010	1.000 45.47
ANISOU 343	CG GLU 43	5175 7105	5377	-2936 -92 - 289
ATOM 344	CD GLU 43	9.750 35.764	52.826	1.000 46.40
ANISOU 344	CD GLU 43	4506 7977	5145	-3155 548 -1210
ATOM 345	OE1 GLU 43	9.775 36.447	53.880	
ANISOU 345	OE1 GLU 43	8741 7607	4627	1.000 55.20
ATOM 346	OE2 GLU 43	10.706 35.080		-2062 -1002 -669
ANISOU 346	OE2 GLU 43	4592 8930	52.433	1.000 56.77
ATOM 347	N LEU 44	_	8050	-2652 939 -1258
ANISOU 347	N LEU 44		55.426	1.000 22.72
ATOM 348		_	3964	464 -476 - 450
ANISOU 348		5.117 32.592	55.959	1.000 26.76
ATOM 349		4009 1973	4187	140 570 - 986
ANISOU 349		5.978 31.585		1.000 28.25
ATOM 350		5094 2194	3448	-153 277 -562
ANISOU 350	CG LEU 44	5.284 30.494		1.000 32.03
		5971 2801	3398	-279 1192 - 627
	CD1 LEU 44	4.485 29.535	56.656	1.000 37.95
ANISOU 351	CD1 LEU 44	7665 2239	4514	-1148 2039 - 1403
ATOM 352	CD2 LEU 44	6.302 29.703	58.361	1.000 36.97
ANISOU 352	CD2 LEU 44	7096 2869	4080	1150 2171 1 8 6
ATOM 353	C LEU 44	4.000 33.145	56.841	1.000 31.10
ANISOU 353	C LEU 44	3835 3182	4800	-700 837 -2205
ATOM 354	0 LEU 44	2.913 32.543		1.000 30.19
ANISOU 354	O LEU 44	4402 3299		-1248 870 -2165
ATOM 355	N ALA 45	4.238 34.247		1.000 28.74
ANISOU 355	N ALA 45	2897 2938		-562 710 -2061
ATOM 356	CA ALA 45	3.382 34.751		1.000 27.09
ANISOU 356	CA ALA 45	2716 2817	4761	-751 467 -2140
ATOM 357	C ALA 45	1.943 35.014		1.000 24.95
ANISOU 357	C ALA 45	2697 3110	3673	-784 709 -1257
ATOM 358	O ALA 45	1.021 34.515		1.000 22.50
ANISOU 358	O ALA 45	2762 2585	3201	
ATOM 359	CB ALA 45	3.975 36.005	59.248	-565 560 -1146
ANISOU 359	CB ALA 45	3259 4219		1.000 36.30
ATOM 360	N SER 46		6315	-1912 1332 - 3404
ANISOU 360	N SER 46	1.729 35.779		1.000 26.85
ATOM 361		3258 3756	3187	-1732 618 -1184
ANISOU 361		0.380 36.052		1.000 24.97
ATOM 362		3686 3189	2611	-1223 511 -1105
ANISOU 362	CB SER 46	0.422 36.950	•	1.000 32.35
	CB SER 46	5428 3467	3395	-2232 70 - 458
_	OG SER 46	0.630 38.289		1.000 45.77
ANISOU 363	OG SER 46	7730 3349	6313	-2746 2499 - 807
ATOM 364	C SER 46	-0.408 34.787	56.307	1.000 20.63
ANISOU 364	C SER 46	2797 2469	2572	-423 -151 - 542
ATOM 365	O SER 46	-1.578 34.672	56.698	1.000 21.93
ANISOU 365	O SER 46	3120 2486	2725	-559 305 -403
ATOM 366	N ALA 47	0.211 33.855	55.590	1.000 22.39
ANISOU 366	N ALA 47	3096 2167	3244	-488 394 <b>-</b> 368
		2101	7644	-400 J2# -708

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ATOM 36	67 CA	ALA 47	-0.397	32.596	55.176	1.000 19.54
ANISOU 36	67 CA	ALA 47	2746	1863	2814	-289 362 - 18
ATOM 36	68 CB	ALA 47	0.548	31.900	54.191	1.000 23.54
	68 CB	ALA 47	3524	1717	3705	-617 1237 - 159
	69 C	ALA 47	-0.715	31.714	56.381	
	69 C	ALA 47				1.000 19.95
			2282	2546	2752	-327 19 2 5 7
		ALA 47	-1.836	31.199	56.518	1.000 19.66
	70 0	ALA 47	2489	2589	2393	-614 211 -165
	71 N	LYS 48	0.270	31.558	57.268	1.000 18.24
	71N	LYS 48		1966	2253	-210 -139 - 912
	72 CA	LYS 48	0.042	30.782	58.486	1.000 19.33
	72 CA	LYS 48	2398	2625	2321	43 -312 - 563
	73 C	LYS 48	-1.110	31.329	59.322	1.000 20.57
	73 C	LYS 48	2476	2556	2785	-326 83 - 566
ATOM 37	74 0	LYS 48	-2.022	30.613	59.771	1.000 20.34
ANISOU 37	74 0	LYS 48	3207	2598	1923	-521 139 -340
ATOM 37	75 CB	LYS 48	1.352	30.758	59.294	1.000 24.61
ANISOU 37	75 CB	LYS 48	2400	3792	3158	-258 -556 - 80
ATOM 37	76 CG	LYS 48	1.237	29.873	60.531	1.000 30.84
ANISOU 37	76 CG	LYS 48	4306	4044	3366	-291 -1504.277
	77 CD	LYS 48	1.837	30.575	61.736	1.000 41.45
	77 CD	LYS 48	6742	5755	3251	-1067 -1382 - 356
	78 CE	LYS 48	1.625	29.717	62.966	1.000 41.63
ANISOU 37		LYS 48	6620	6124	3073	-466 -1047 - 353
	79 NZ	LYS 48	1.074	30.497	64.112	1.000 42.62
	79 NZ	LYS 48	5883	6866	3444	460 -1193 - 425
	80 N	ASP 49	~1.110	32.625	59.607	1.000 19.18
	80 N		= 2348	2602	2337	
	81 CA	ASP 49	-2.127	33.243		-464 100 -806 1 000 31 05
	81 CA	ASP 49			60.433	1.000 21.95
	82 CB	ASP 49		2986 34.756	2801	-791 617 <b>-</b> 1035
	82 CB		-1.868		60.611	1.000 23.97
	83 CG			2872	3409	-250 -79 -1325
		ASP 49	-0.681	35.078	61.492	1.000 25.41
	_	ASP 49		3405	3464	-365 113 -1866
				34.153	62.143	
	84 OD1			4181.	3932	-254 -967 -1667
	85 OD2				61.563	
	85 OD2			3649	4742	-710  344  -2413
	86 C	ASP 49		33.061	59.904	1.000 21.44
	86 C	ASP 49		2651	3030	-388 540 -900
	87 0	ASP 49		32.770	60.654	1.000 20.72
	87 0	ASP 49		2181	3347	-279 550 -726
	88 N	LEU 50			58.596	1.000 23.28
	88 N	LEU 50		2712	3191	$-1251\ 216\ -644$
	89 CA	LEU 50		33.185	58.068	1.000 22.94
	89 CA	LEU 50		1796	3815	-575 -205 -1079
	90 CB	LEU 50			56.696	1.000 28.78
ANISOU 3	- ·	LEU 50	3948	2453	4535	-852 -755 - 254
	91 CG	LEU 50	-6.620	34.246	56.260	1.000 25.30
	91 CG	LEU 50	3800	2294	3520	30 325 - 5 3 1
		LEU 50	-7.552	34.478	57.441	
ANISOU 3	92 CD1	LEU 50	6382	4432	6196	-475 3026 - 1060
ATOM 3	93 CD2	LEU 50		35.485	55.385	
ANISOU 3	93 CD2	LEU 50	<del>_</del>	1962	4533	752 354 - 433
ATOM 3	94 C	LEU 50		31.737	57.982	1.000 21.12
ANISOU 3	94 C	LEU 50		1870	3595	-643 742 -1270
ATOM 3	95 0	LEU 50	·	31.494		1.000 21.13
	95 0	LEU 50	=	2457	3083	-543 579 -1097
	96 N	VAL 51		30.769		
ANISOU 3		VAL 51		1843	1823	-302 -3 -646
	97 CA	VAL 51				

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ANISOU 397 CAVAL 3154 51 1763 -401 -15 -4271947 398 MOTA CBVAL 51 -4.281 28.415 56.889 1.000 16.07 ANISOU 398 CB 51 VAL 2981 1629 1496 -621 -255 - 501 MOTA 399 CG1 VAL 51 -3.002 28.114 57.668 1.000 18.99 ANISOU 399 CG1 VAL 51 2959 1875 2382 -383 -100 3 0 2 ATOM CG2 VAL 400 51 -5.006 27.119 56.497 1.000 22.16 ANISOU 400 CG2 VAL 51 4569 1728 -1393 64 - 869 2121 ATOM 401 C VAL 51 -5.446 28.899 59.114 1.000 17.74 ANISOU 401 C VAL 51 2508 2223 2009 142 - 445 -435 ATOM 402 VAL 51 -6.43059.346 28.187 1.000 19.76 ANISOU 402 0 VAL 51 3005 2160 2345 726 -1021 -692 ATOM 403 ILE 52 M -4.67129.263 60.125 1.000 20.23 ANISOU 403 N ILE 52 2980 2945 1760 364 - 902 -649 ATOM 404 CA ILE 52 -4.990 28.875 61.507 1.000 20.17 ANISOU 404 ILE 52 2665 CA3200 1800 627 -1134 -758 MOTA 405 CB ILE 52 -3.84729.230 62.469 1.000 21.31 ANISOU 405 CB ILE 52 3294 3151 -449 462 -1043 1652 CG2 ILE ATOM 406 52 -4.238 63.931 1.000 21.29 29.178 CG2 ILE ANISOU 406 52 3543 2826 1719 -362 529 -689CG1 ILE -2.619 ATOM 407 52 28.346 62.217 1.000 25.37 CG1 ILE ANISOU 407 52 3819 3213 2608 -307 727 -1090ATOM CD1 ILE 408 52 -2.87162.470 1.000 28.56 26.872 ANISOU 408 CD1 ILE 52 3474 3578 3798 106 178 -1110 ATOM 409 ILE C 52 -6.28429.514 61.950 1.000 22.44 ANISOU 409 ILE C 52 3119 645 -1228 3216 2190 -710 ATOM 410 ILE 52 0 -7.072 28.856 62.647 1.000 23.23 ANISOU 410 0 ILE 52 3390 3654 1781 -766 758 -1246 ATOM 411 ASP N53 .-6.519 30.754 61.530 1.000 23.33 ANISOU 411 ASP N 53 2897 -626 700 -1361 3064 2903 ATOM 412 CA ASP 53 -7.82631.335 61.897 1.000 24.49 ANISOU 412 ASP CA53 2818 3347 3141 -759 781 -1545 ATOM CB413 ASP 53 -7.94232.781 61.411 1.000 27.43 ANISOU 413 CB ASP 53 2854 3335 -434 819 -1446 4235 ATOM 414 ASP CG 53 -9.309 61.570 33.397 1.000 30.99 ANISOU 414 ASP CG 53 3166 4281 4326 36 1242 -1214 ATOM 415 OD1 ASP 53 -9.657 33.779 62.705 1.000 37.26 ANISOU 415 OD1 ASP 4569 53 4369 5220 153 1263 - 2733 ATOM 416 OD2 ASP 53 -10.050 33.491 60.553 1.000 38.45 ANISOU 416 OD2 ASP 53 3393 5173 6043 810 557 - 1648 ATOM 417 ASP 53 C -8.953 61.316 1.000 24.64 30.495 ANISOU 417 ASP C 53 3028 3701 2634 -919 372 -1031 ATOM 418 -10.011 30.327 61.915 1.000 28.52 ASP 53 ANISOU 418 ASP 53 O 3399 -1519 962 -2151 3835 3603 ATOM 419  $\mathbf{N}$ PHE 29.978 60.108 1.000 22.04 54 -8.744ANISOU 419 PHE N 54 2921 2974 2479 -573 174 -704ATOM 420 CA . 54 PHE -9.772 29.187 59.432 1.000 19.99 ANISOU 420 CAPHE 54 2253 2879 2463 -421 771 - 978 ATOM 421 PHE CB 54 -9.423 29.030 57.942 1.000 18.45 ANISOU 421 PHE CB54 2856 1983 2171 -65 426 - 518 ATOM 422 CG PHE -10.493 28.292 54 57.145 1.000 21.36 ANISOU 422 PHE CG 54 3063 2735 2318 -646 599 -627MOTA CD1 PHE 423 54 -11.714 28.906 56.933 1.000 23.18 CD1 PHE ANISOU 423 54 2783 3199 2826 -703 -29 -624CD2 PHE ATOM 424 -10.293 27.035 54 56.619 1.000 23.32 ANISOU 424 CD2 PHE 54 3482 2802 -689 212 -858 2577 CE1 PHE ATOM 425 54 -12.719 28.291 56.241 1.000 26.45 CE1 PHE ANISOU 425 54 3696 3345 3008 -1418129 - 554CE2 PHE ATOM 426 -11.303 26.375 55.921 1.000 25.65 54 CE2 PHE ANISOU 426 54 3750 3815 -1404607 - 10052182 ATOM 427 CZPHE 54 -12.522 27.013 55.725 1.000 26.17 ANISOU 427 CZPHE 54 3433 3830 2679 -1829298 - 813

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MOTA
       428
                                 27.854
            C
                PHE
                     54
                         -9.959
                                         60.132 1.000 19.44
ANISOU 428
            C
                     54
                PHE
                         2340
                                  3430
                                          1617
                                                  -834
                                                        319 - 759
       429
                         -11.087 27.450
ATOM
                     54
            0
                PHE
                                         60.386 1.000 22.11
ANISOU 429
                PHE
            0
                     54
                                  3066
                         2601
                                          2734
                                                 -948 1018 - 1466
       430
ATOM
                PHE
            N
                     55
                         -8.882
                                 27.166
                                         60.448 1.000 20.59
ANISOU 430
                PHE
                     55
            N
                         2728
                                  3375
                                                 -666 180 -611
                                          1720
            CA
                PHE
                                 25.927
ATOM
       431
                     55
                         -8.966
                                          61.212
                                                 1.000 22.59
                PHE
                                  3671
ANISOU 431
                     55
            ÇA
                         3092
                                          1820
                                                 -728 381 -372
ATOM
       432
                PHE
            CB
                     55
                         -7.579
                                 25.360
                                          61.478
                                                 1.000 21.93
ANISOU 432
                     55
            CB
                PHE
                         3163
                                  3622
                                                 -692 287 -158
                                          1549
                PHE
ATOM
       433
            CG
                     55
                         -6.790
                                          60.284 1.000 20.60
                                 24.833
            CG
ANISOU 433
                PHE
                     55
                         3034
                                  2998
                                          1793
                                                 -1004365 - 375
       434
                     55
            CD1 PHE
ATOM
                         -7.352
                                 24.526
                                         59.057 1.000 18.72
ANISOU 434
            CD1 PHE
                     55
                         2300
                                  3095
                                                 -1078 586 -271
                                          1717
            CD2 PHE
MOTA
       435
                     55
                         -5.430
                                          60.385 1.000 18.06
                                  24.615
ANISOU 435
            CD2 PHE
                     55
                         3132
                                  2490
                                          1241
                                                 -926 128 -497
            CE1 PHE
       436
ATOM
                     55
                         -6.609
                                          58.014 1.000 18.92
                                 24.037
            CE1 PHE
ANISOU 436
                     55
                         2455
                                  2761
                                          1971
                                                 -844 436 -542
MOTA
       437
            CE2 PHE
                     55
                         -4.672
                                 24.124
                                         59.352 1.000 18.58
            CE2 PHE
ANISOU 437
                     55
                         3291
                                  2606
                                          1163
                                                 -478
                                                       63 - 299
       438
ATOM
            CZ
                PHE
                     55
                         -5.256
                                 23.814
                                         58.134 1.000 17.68
ANISOU 438
            CZ
                PHE
                     55
                         2660
                                  2567
                                          1490
                                                 -380 129 - 806
       439
            C
ATOM
                     55
                PHE
                         -9.684
                                 26.111
                                          62.546 1.000 24.99
ANISOU 439
                PHE
                                  4138
            C
                     55
                         3310
                                          2046
                                                 -830 647 -415
                         -10.532 25.281
ATOM
       440
                PHE
                     55
            0
                                          62.872 1.000 30.29
                PHE
ANISOU 440
                     55
            0
                         3802
                                  4943
                                          2763
                                                 -1527 1314 - 1102
ATOM
       441
                GLU
            N
                     56
                         -9.330
                                 27.144
                                          63.311 1.000 23.65
ANISOU 441
                GLU
                        2864
                     56
            N
                                  4109
                                          2013
                                                 -634 937 -525
ATOM
       442
                     56
                                 27.355
            CA
                GLU
                                          64.636 1.000 30.01
                         -9.868
ANISOU 442
            CA
                GLU
                     56
                         3632
                                  5378
                                          2394
                                                  -1050 1465 - 9 9 4
                     56
ATOM
       443
            CB
                GLU
                         -8.998
                                  28.333
                                          65.436 1.000 36.40
ANISOU 443
            CB
                GLU
                     56
                                  6933
                         4531
                                          2367
                                                  -1606 1318 - 1623
ATOM
       444
            CG
                     56
                GLU
                                  27.827
                         -7.666
                                          65.916 1.000 41.89
ANISOU 444
            CG
                GLU
                     56
                         5006
                                  8196
                                                  -1457404 - 1900
                                          2713
ATOM
       445
            CD
                GLU
                     56
                         -6.787
                                          66.575 1.000 48.94
                                  28.880
ANISOU 445
            CD
                GLU
                     56
                         6081
                                  9310
                                          3202
                                                  -2278 -73 -2062
ATOM
       446
            OE1 GLU
                     56
                         -5.694
                                  28.515
                                          67.078 1.000 60.73
ANISOU 446
            OE1 GLU
                     56
                         8034
                                  12274
                                          2769
                                                  -3208 -2335 2 6 6
ATOM
       447
            OE2 GLU
                    56
                                 30.084 66.614 1.000 58.51
                         -7.145
ANISOU 447
            OE2 GLU
                    56
                          8742
                                          4151
                                  9338
                                                  -2088 1096 - 3951
            C GLU 56 -11.289 27.920 64.617 1.000 30.60
ATOM 448
ANISOU 448 · C
                    56
                GLU
                         3764
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                                          2941
                                                  -977 1967 - 1271
ATOM
       449
                         -12.058 27.542 65.504 1.000 35.21
                    56
                GLU
ANISOU 449
                GLU
                     56
                         4384
                                  5304
                                          3690
                                                  -1136 2652 - 1235
                         -11.603 28.805
ATOM
       450
                HIS
                                          63.673 1.000 30.00
            N
                     57
ANISOU 450
                HIS
            N
                     57
                         3730
                                  4846
                                          2823
                                                  -654 1684 - 1582
       451
ATOM
                HIS
                     57
            CA
                         -12.854 29.559
                                          63.759 1.000 33.51
ANISOU 451
                HIS
                     57
            CA
                         3853
                                  5101
                                          3778
                                                  -519 1673 - 1911
       452
ATOM
                HIS
            CB
                     57
                          -12.536 31.046
                                          63.991 1.000 33.40
ANISOU 452
            CB
                                                  -411 1546 - 2250
                HIS
                     57
                          3844
                                  5183
                                          3664
ATOM
       453
                HIS
                          -11.577 31.344
            CG
                     57
                                          65.095 1.000 35.13
ANISOU 453
               HIS
                     57
            CG
                          4497
                                  5409
                                          3444
                                                  -505 1340 - 1992
ATOM
       454
            CD2 HIS
                          -10.361 31.946
                                          65.071 1.000 35.26
                     57
ANISOU 454
            CD2 HIS
                     57
                         4837
                                  5214
                                          3345
                                                  -834 637 -1456
ATOM
       455
            ND1 HIS
                          -11.819 31.021
                     57
                                          66.411 1.000 40.52
ANISOU 455
            ND1 HIS
                     57
                          6021
                                                  -1360 1474 - 2002
                                          3490
                                  5885
            CE1 HIS
ATOM
       456
                          -10.798 31.410 67.151 1.000 42.28
                     57
ANISOU 456
            CE1 HIS
                                  6066
                      57
                          6680
                                          3320
                                                  -1632 1099 - 1772
ATOM
       457
                         -9.902 31.970 66.362 1.000 41.69
            NE2 HIS
                     57
ANISOU 457
            NE2 HIS
                      57
                         6377
                                  6133
                                          3329
                                                  -1817 407 -1148
ATOM
       458
                HIS
                          -13.769 29.466 62.547 1.000 32.58
            C
                     57
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						100 -		
ANISOU	458	С	HIS	57	3083	5097	4199	-729 1723 - 2066
ATOM	459	0	HIS	57	-14.902	29.965	62.578	1.000 33.80
ANISOU	459	0	HIS	57	3121	5097		
ATOM	460	N	GLY	58			4625	-731 1865 - 2565
ANISOU		N				28.866	61.432	1.000 28.78
			GLY	58	2841	4353	3742	-253 1341 -1506
ATOM	461	Că	$\mathtt{GLY}$	58	-14.326	28.685	60.332	1.000 26.99
ANISOU	461	C 5	${ t GLY}$	58	2471	3916	3869	24 1298 -1173
ATOM	462	С	GLY	58	-15.447		60.738	
ANISOU	462	С	GLY	58	2665			1.000 29.94
ATOM	463	Ö	GLY	58		4357	4353	-261 1323 - 1058
ANISOU					-15.241		61.534	1.000 29.23
		0	GLY	58	2976	4044	4087	-571 1192 - 1297
ATOM	464	N	SER	59	-16.635	27.958	60.193	1.000 27.61
ANISOU	464	N	SER	59	2556	3905	4029	-108 1461 - 1767
ATOM	465	CA	SER	59	-17.812		60.497	
ANISOU	465	CA	SER	59	2675	4074		1.000 28.42
ATOM	466	CB	SER	59			4049	-189 1294 -1325
ANISOU					-19.121		60.162	1.000 28.29
		CB	SER	59	2556	4574	3618	-339 1198 - 928
ATOM	467	0G	SER	59	-19.229	27.978	58.739	1.000 28.66
ANISOU		OG	SER	59	3598	3742	3547	166 1729 - 867
MOTA	468	C	SER	59	-17.795		59.724	
ANISOU	468	С	SER	5 9	3467	3990		1.000 29.57
ATOM	469	0	SER	59			3779	-646 1463 -1206
ANISOU		Ö			-16.990		58.810	1.000 22.72
			SER	59	3054	3042	2537	-144 648 - 369
ATOM	470	N	GLU	60	-18.698	24.939	60.103	1.000 26.90
ANISOU		N	GLU	60	2413	3900	3907	-69 1079 - 853
ATOM	471	CA	GLU	60	-18.699		59.359	
ANISOU	471	CA	GLU	60	2699	3515		
ATOM	472	CB	GLU	60	•		4037	<b>-98 709 -537</b>
ANISOU		CB	GLU		-19.646		60.001	
ATOM					5393	4393	5075	-1361 908 3 6 4
	473	CG	GLU	60	-19.011	21.665	60.917	1.000 44.63
ANISOU		CG	GLU	60	5606	5473	5878	-977 1079 1219
ATOM	474	CD	GLU	60	-17.507	21.543		1.000 48.52
ANISOU	474	CD	GLU	60	5714	6217	6503	
ATOM	475	OE1	GLU	60	-17.030			
ANISOU	475		GLU	60	5349		59.684	1.000 48.11
ATOM	476		GLU			7545	5384	709 366 1951
ANISOU				60	-16.828		61.829	1.000 46.50
=	_	OE2	GLU	60	4926	5742	7000	1158 1550 - 1504
ATOM	477	С	GLU	60	-19.091	23.960	57.915	1.000 25.30
ANISOU	477	С	GLU	60	2829	2728	4055	86 725 - 656
ATOM	478	0	GLU	60	-18.529		57.027	
ANISOU	478	0	GLU	60	2119	2980	4091	
ATOM	479	N	ALA	61				-202 741 - 752
ANISOU	479	N	ALA	61	-20.032		57.716	
ATOM	480				2083	3206	4432	-34 612 $-774$
		CA	ALA	61	-20.495		56.368	1.000 24.05
ANISOU	_	CA	ALA	61	1838	2999	4301	228 720 -1055
MOTA	481	CB	ALA	61	-21.670	26.176	56.459	1.000 27.53
ANISOU	481	CB	ALA	61	2807	1857	5797	
ATOM	482	С	ALA	61	-19.385		_	
ANISOU	482	C	ALA	61				1.000 27.31
ATOM	483	0			3170	2572	4633	-377 1178 -1026
			ALA	61	-19.247	25.467	54.311	1.000 22.29
ANISOU		0	ALA	61	2363	1876	4232	42 661 - 319
ATOM	484	N	GLU	62	-18.580	26.642		1.000 22.18
ANISOU	484	N	GLU	62	2075	2258	4094	
ATOM	485	CA	GLU	62				396 569 - 394
ANISOU		CA	GLU	62	11.4JD			1.000 24.19
ATOM	486				2401	2603	4188	150 852 - 590
		CB	GLU.	62	-16.806	28.354	56.277	1.000 24.68
ANISOU		CB	GLU	62	2401	2490	4485	91 1273 -828
ATOM	487	CG	GLU	62	-17.641	29.636	56.356	1.000 25.19
ANISOU	487	CG	GLU	62	2542	2620	4409	
ATOM	488	CD	GLU	62	-17.288			
ANISOU		CD	GLU	62			57.480	1.000 29.27
		~ <i>~</i>		J 2	3284	2991	4845	621 515 -1290

ATOM 489	OE1 GLU	62	-16.527	30 2/1	58.410	1.000 30.11
ANISOU 489	OE1 GLU	62		3067	5143	318 56 - 1639
ATOM 490	OE2 GLU	62	-17.796		57.436	1.000 35.30
ANISOU 490 ATOM 491	OE2 GLU C GLU	62	4832	2994	5584	863 109 -1327
ANISOU 491	C GLU C GLU	62 62		26.226	55.025	1.000 21.70
ATOM 492	O GLU	62	-15.818	2421	3430 53.940	30 784 - 579 1.000 19.44
ANISOU 492	O GLU	62		2140	3153	-301 467 -604
ATOM 493	N LYS	63	-16.184		55.972	1.000 20.08
ANISOU 493	N LYS	63		2266	2893	-74 761 -902
ATOM 494 ANISOU 494	CA LYS	63 63	-15.246		55.678	1.000 19.73
ATOM 495	CB LYS	63	2322 -14.934	2559 23 497	2614 56.988	133 429 - 903 1.000 18.48
ANISOU 495	CB LYS	63		2743	2476	-218 587 -836
ATOM 496	CG LYS	63	-13.946		57.881	1.000 19.17
ANISOU 496	CG LYS	63		2332	2836	-296 325 -674
ATOM 497 ANISOU 497	CD LYS	63 63	-13.839 2978		59.290	1.000 26.23
ATOM 498	CE LYS	63		4084 24.383	2902 60.068	-888 -177 - 287 1.000 27.75
ANISOU 498	CE LYS	63	3074	5008	2461	-1239 500 -1082
ATOM 499	NZ LYS	63	-12.929		61.530	1.000 34.95
ANISOU 499 ATOM 500	NZ LYS C LYS	63	3177	7579	2524	-2594 840 - 894
ANISOU 500	C LYS	63 63	-15.789 2014	23.304 2191	54.586 2453	1.000 17.52 51 529 - 691
ATOM 501	O LYS	63	-15.025		53.654	1.000 17.58
ANISOU 501	O LYS	63	2266	1709	2704	158 707 - 653
ATOM 502 ANISOU 502	N ARG N ARG	64	-17.069		54.641	1.000 19.63
ATOM 503	N ARG CA ARG	64 64	2081 -17.618	2452	2926 53.595	-14 614 $-592$ 1.000 19.00
ANISOU 503	CA ARG	64	1509	2526	3185	-3 620 - 652
ATOM 504	C ARG	64	-17.471		52.194	1.000 20.42
ANISOU 504 ATOM 505	C ARG	64	2165	2436	3157	-390 -22 -536
ATOM 505 ANISOU 505	O ARG O ARG	64 64	-17.204 $1854$	21.934 2184	51.195 3115	1.000 18.83 -434 575 - 201
ATOM 506	CB ARG	64			53.871	1.000 24.70
ANISOU 506	CB ARG	64	1470	3652	4263	-51 841 - 909
ATOM 507	CG ARG	64	-19.838		52.795	1.000 36.49
ANISOU 507 ATOM 508	CG ARG	64 64	2961 -21.315	5284	5621 53.095	-2020 138 - 882
ANISOU 508	CD ARG	64	3034	6962	7603	1.000 46.32 -2438 327 -1187
ATOM 509	NE ARG	64	-21.776		54.331	1.000 55.81
ANISOU 509	NE ARG	64	3917	8636	8652	-3960 2222 -1870
ATOM 510 ANISOU 510	CZ ARG	64 64	-22.814 4438			1.000 58.82
ATOM 511	NH1 ARG	64	-23.884	8939	8972 54.071	-3479 1988 - 2480 1.000 76.83
ANISOU 511	NH1 ARG	64	6024	9527	13641	-1787 -165 - 1872
ATOM 512	NH2 ARG	64	-22.797	22.213		1.000 69.53
ANISOU 512	NH2 ARG	64	7792	9201		-5884 3891 - 3 3 0 4
ATOM 513 ANISOU 513	N ALA N ALA	65 65	-17.621 1689	23.947	52.066 3519	1.000 20.43 24 612 -525
ATOM 514	CA ALA	65	-17.505			
ANISOU 514	CA ALA	65	1649	2216	3523	409 184 - 553
ATOM 515	CB ALA	65	-17.912			
ANISOU 515 ATOM 516	CB ALA C ALA	65 65	1420 -16.118	2019	5579 50.168	126 -373 - 742
ANISOU 516	C ALA	65	1524	24.549	3173	1.000 17.89 -47 108 -101
ATOM 517	O ALA	65	-15.983		48.954	
ANISOU 517	O ALA	65	1830	2178	3123	122 -8 -229
ATOM 518 ANISOU 518	N VAL N VAL	66 66	-15.100			1.000 17.99
ATOM 519	CA VAL	66 66	1547 -13.746	2151	3137 50.430	-86 36 - 196 1.000 16.74
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ANISOU 519 CA VAL 66 1553 1859 2948 -56 - 254-62 520 -12.775 25.151 MOTA VAL CВ 66 50.951 1.000 17.29 ANISOU 520 CB VAL 66 1805 1804 2963 -330 338 -185 CG1 VAL 521 ATOM -13.238 26.532 66 1.000 16.70 50.455 ANISOU 521 CG1 VAL 1547 66 1800 2997 111 545 - 553CG2 VAL 522 MOTA 66 -12.652 25.180 52.462 1.000 18.65 CG2 VAL ANISOU 522 2053 66 1995 3036 -193 17 - 538 MOTA 523 C VAL -13.201 22.680 66 50.724 1.000 15.66 ANISOU 523  $\mathsf{C}$ VAL 66 1775 1813 2362 -70 -250 - 457524 MOTA 0 VAL -11.972 22.493 50.808 66 1.000 14.19 ANISOU 524 0 VAL 66 1747 1576 2069 -56 -347 -122 525 ATOM THR N -14.071 21.695 67 50.873 1.000 14.46 ANISOU 525 N THR 67 1550 1602 2343 126 -48 -722 526 ATOM THR CA67 -13.723 20.279 51.000 1.000 14.06 ANISOU 526 CA THR 67 1698 1461 2185 234 5 - 740ATOM 527 CB THR 67 -14.419 19.647 52.225 1.000 15.08 ANISOU 527 CB THR 67 1721 1955 2053 -51 -426 - 444 528 ATOM OG1 THR -14.089 20.337 67 53.453 1.000 17.41 ANISOU 528 OG1 THR 67 2538 1949 2128 70 - 716 -39 529 CG2 THR ATOM -13.915 18.215 67 52.420 1.000 16.63 ANISOU 529 CG2 THR 67 2182 1888 2248 148 293 - 658 530 MOTA THR -14.067 19.518 C 67 49.728 1.000 12.37 ANISOU 530 C THR 67 1144 1422 2132 209 -95 - 517ATOM 531 0 THR 67 -15.208 19.567 49.229 1.000 14.82 ANISOU 531 THR 0 67 1197 2086 2350 208 -168 - 362ATOM 532 -13.092 18.790 N SER 68 49.180 1.000 11.61 ANISOU 532 N 68 SER 1109 1421 1881 37 - 58 - 534 MOTA 533 SER CA68 -13.306 17.955 48.003 1.000 11.45 ANISOU 533 CA 68 <sup>2</sup> 1274 SER 1444 1631 -49 -30 - 374ATOM 534 CBSER -12.027 17.317 68 47.480 1.000 11.88 ANISOU 534 CB 1446 SER 68 1523 1544 79 252 - 157 535 ATOM -11.026 18.292 OG SER 68 47.239 1.000 16.95 ANISOU 535 SER OG 68 1557 2314 2569 -336 389 - 218 ATOM 536 C SER -14.269 16.815 68 48.319 1.000 11.56 ANISOU 536 C SER 1287 68 1375 1732 53 - 406 -61 ATOM 537 0 -14.308 16.384 SER 68 49.476 1.000 14.62 ANISOU 537 0 SER 68 1998 1860 -538 153 -430 1697 538 ATOM N 69 -15.026 16.324 PRO 47.344 1.000 12.78 ANISOU 538 N PRO 1476 69 1473 1905 -243 -88 - 194ATOM 539 CD PRO -15.130 16.801 69 45.953 1.000 12.47 ANISOU 539 CD PRO 69 1022 1808 -199 -203 -1441909 ATOM 540 CAPRO 69 47.639 1.000 12.21 -15.941 15.214 ANISOU 540 CA PRO 1358 69 1369 -178. 148 -437 1913 ATOM 541 CB PRO -16.825 15.193 69 46.355 1.000 13.94 ANISOU 541 CB PRO 69 1362 1591 2343 -251 - 178 - 14ATOM 542 -15.924 15.715 CG PRO 69 45.290 1.000 14.38 ANISOU 542 CG PRO 69 1396 1947 2122 -554 -511 1 7 8 ATOM 543 C PRO -15.270 13.882 69 47.912 1.000 13.25 ANISOU 543 C PRO 69 1206 1526 2303 -217 -115 -100ATOM 544 -15.932 12.985 0 PRO 69 48.481 1.000 14.01 ANISOU 544 0 PRO 69 1753 2122 -373 99 -3011450 ATOM 545 VAL -14.015 13.692 N 70 47.554 1.000 13.46 ANISOU 545 NVAL 70 1288 1479 2348 -174 -108 - 265 ATOM 546 -13.184 12.548 CAVAL 70 47.898 1.000 13.49 ANISOU 546 CAVAL 70 1404 1692 2030 37 138 - 195 547 ATOM -12.587 11.720 CB VAL 70 46.737 1.000 16.39 ANISOU 547 CB VAL 70 2142 1648 2439 -225 614 -452 548 MOTA CG1 VAL -13.615 10.756 70 46.208 1.000 33.50 ANISOU 548 CG1 VAL 70 6470 2984 3274 -2702 41 - 867 CG2 VAL ATOM 549 -11.995 12.613 45.640 1.000 16.46 70 ANISOU 549 CG2 VAL 70 1749 2234 2273 269 444 2 3

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ATOM
       550
            C
                VAL
                         -12.042 13.057
                                          48.782 1.000 13.59
                     70
ANISOU 550
            C
                         1618
                VAL
                     70
                                          2163
                                  1382
                                                  -38
                                                        -114 1 2 7
MOTA
       551
                         -11.426 14.105
                                          48.493
            0
                VAL
                     70
                                                  1.000 14.20
ANISOU 551
                     70
                VAL
                          1748
                                  1685
                                          1964
                                                  -265
                                                        26 1 8 2
ATOM
       552
                     71
            N
                PRO
                         -11.786 12.365
                                          49.898
                                                  1.000 14.21
ANISOU 552
                                          2285
                PRO
                     71
                         1607
                                  1507
                                                  -115 -62 310
            Ν
       553
            CD
                          -12.432 11.125
ATOM
                PRO
                     71
                                          50.378
                                                  1.000 14.70
ANISOU 553
            CD
                PRO
                     71
                         1920
                                  1590
                                          2076
                                                  -201
                                                        646 4
ATOM
       554
                PRO
                     71
            ÇA
                          -10.830 12.919
                                          50.878
                                                  1.000 17.41
ANISOU 554
                          2429
            CA
                PRO
                     71
                                  2008
                                                       -342 4 1 8
                                          2178
                                                  -522
                          -11.338 12.304 52.193 1.000 20.87
                     71
ATOM
       555
            CB
                PRO
ANISOU 555
            CB
                PRO
                     71
                         3768
                                  2082
                                          2081
                                                  -743 190 1 4
            CG
                     71
                         -11.908 10.989
       556
                                          51.775 1.000 18.28
ATOM
                PRO
ANISOU 556
                PRO
            CG
                         3534
                     71
                                  1665
                                          1746
                                                  -338
                                                       781 - 54
       557
ATOM
                          -9.384
                                  12.543
            C
                PRO
                     71
                                          50.619 1.000 17.14
ANISOU 557
                PRO
            C
                         2183
                     71
                                  2304
                                          2026
                                                  -684
                                                        -815 4 4
       558
                     71
                         -8.730
ATOM
            0
                PRO
                                  11.796
                                          51.330 1.000 20.54
ANISOU 558
                PRO
                     71
            0
                          2745
                                          2448
                                                  -87
                                  2610
                                                        -404 4 1 4
       559
ATOM
            N
                THR
                     72
                          -8.834
                                  13.111
                                          49.556 1.000 16.59
ANISOU 559
            N
                THR
                     72
                          2156
                                  2046
                                          2103
                                                  -235
                                                        -508 - 17
ATOM
       560
            CA
                THR
                     72
                          -7.496
                                  12.818
                                         49.090 1.000 17.43
ANISOU 560
                     72
            CA
                THR
                          2113
                                  1884
                                          2626
                                                  -254 -510 -288
            CB
       561
                     72
                          -7.477
ATOM
                THR
                                  12.829
                                          47.545 1.000 15.98
ANISOU 561
            CB
                THR
                     72
                          1700
                                  1761
                                          2611
                                                  211
                                                        -458 - 421
       562
                                  14.094
            OG1 THR
                                          47.128 1.000 17.28
MOTA
                          -8.027
                     72
            OG1 THR
ANISOU 562
                     72
                          2146
                                  1553
                                          2868
                                                  27 - 355 - 271
            CG2 THR
ATOM
       563
                     72
                          -8.348
                                  11.764
                                          46.929
                                                  1.000 12.63
ANISOU 563
                     72
            CG2 THR
                        1296
                                  1581
                                          1923
                                                  -46
                                                        328 - 127
                         -6.418
       564
                THR
                     72
                                          49.549 1.000 17.83
ATOM
            C
                                  13.805
            C
                THR
ANISOU 564
                     72
                          2153
                                  1773
                                          2847
                                                  -155 -1228 2 3 2
       565
ATOM
                     72
                          -5.216
            0
                THR
                                          49.329
                                                 1.000 20.17
                                  13.536
ANISOU 565
                THR
                     72
            0
                                  2265
                                                  -225
                          2142
                                          3257
                                                        -1049 4 8 0
       566
                      73
                          -6.785
ATOM
            N
                MET
                                  14.920
                                          50.169 1.000 19.43
ANISOU 566
            N
                MET
                      73
                          2876
                                          2455
                                                  -782 -451 - 144
                                  2052
ATOM
       567
            CA
                MET
                      73
                          -5.799
                                  15.944
                                          50.521 1.000 18.75
ANISOU 567
            CA
                MET
                      73
                          2117
                                          2682
                                                  -538 -466 - 280
                                  2326
       568
ATOM
            CB
                MET
                      73
                                  15.338
                                          51.480 1.000 22.03
                          -4.758
ANISOU 568
                                                        -306 5 9 5
            CB
                MET
                      73
                          1826
                                  2825
                                          3718
                                                  -377
                      73
ATOM
       569
            CG
                MET
                          -5.374
                                  15.059
                                          52.843 1.000 27.01
            CG
ANISOU 569
                MET
                      73
                          3545
                                  2853
                                          3864
                                                         -87 1526
                                                  -84
MOTA
       570
                     73 -4.107 14.850 54.107 1.000 32.23
                MET
            SD
ANISOU 570
            SD
                MET
                      73
                          4364
                                          3637
                                                  469
                                  4245
       571
                          -3.179 13.492 53.374 1.000 26.74
ATOM
                MET
                      73
            CE
ANISOU 571
            CE
                                  4895
                MET
                      73
                          2885
                                          2381
                                                  326
                                                         425 1348
       572
            C
                MET
                         -5.066
ATOM
                      73
                                  16.582 49.355 1.000 17.20
ANISOU 572
            C
                MET
                      73
                          1338
                                          3067
                                  2129
                                                  -20
                                                        -269 - 175
       573
ATOM
                                  17.110 49.498 1.000 21.20
                MET
                      73
                          -3.945
            0
ANISOU 573
                MET
                      73
                          1713
                                  2512
                                          3832
                                                  -541 51 -1024
            0
                          -5.630 16.600 48.175 1.000 18.64
                 ARG
ATOM
       574
                      74
            N
ANISOU 574
                 ARG
                                  2051
            N
                      74
                          1881
                                          3150 84 - 461 5 4 3
ATOM
       575
                ARG
            CA
                          -5.091
                                  17.180 46.967 1.000 15.73
                      74
ANISOU 575
                ARG
            CA
                      74
                         937 1986
                                       3053
                                               169
                                                     27 - 174
            CB
                 ARG
                         -5.655 16.537 45.704 1.000 16.53
ATOM
       576
                      74
ANISOU 576
                 ARG
             CB
                                                  -263 142 - 160
                     74
                                  1434
                                          3137
                          1711
       577
                         -4.911 16.934 44.440 1.000 15.01
MOTA
            CG
                 ARG
                      74
ANISOU 577
                                                   -156 279 -554
                 ARG
             CG
                          1270
                      74
                                  1288
                                          3144
        578
                                  16.543 43.185 1.000 16.10
MOTA
                 ARG
             CD
                          -5.683
                      74
ANISOU 578
                 ARG
             CD
                          1967
                      74
                                   1031
                                           3120
                                                   268
                                                         -92 - 407
ATOM
        579
                                  16.816 41.966 1.000 18.81
             NE
                 ARG
                      74
                         -4.902
ANISOU 579
                          2259
             NE
                 ARG
                      74
                                   1813
                                           3075
                                                 -432 -252 - 296
        580
ATOM
             CZ
                 ARG
                         -5.033
                      74
                                   17.824 41.130 1.000 16.64
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		10	09 -	
ANISOU 580	CZ ARG 7			-141 -190 - 596
ATOM 581	NH1 ARG 7		.775 41.293	-141 -190 -596 $1.000 20.09$
ANISOU 581	NH1 ARG 7			54 - 353 - 788
ATOM 582	NH2 ARG 7		.896 40.068	1.000 20.12
ANISOU 582 ATOM 583	NH2 ARG 7			153 -196 - 400
ATOM 583 ANISOU 583	C ARG 7 C ARG 7		.681 46.966	1.000 12.70
ATOM 584	O ARG 7		80 1758 .465 46.582	6 -22 - 136 1.000 14.07
ANISOU 584	O ARG 7			-221 -170 - 480
ATOM 585	N ARG 7	5 -6.567 19	.099 47.387	1.000 12.72
ANISOU 585	N ARG 7		— · — •	95 182 - 108
ATOM 586 ANISOU 586	CA ARG 7 CA ARG 7	_	.471 47.308	1.000 13.40
ATOM 587	CB ARG 7		18 1548 .784 45.995	87 275 - 193
ANISOU 587	CB ARG 7			1.000 13.45 -179 51 - 9
ATOM 588	CG ARG 7	5 -6.908 20	.637 44.721	1.000 13.38
ANISOU 588	CG ARG 7	_		78 -217 101
ATOM 589 ANISOU 589	CD ARG 7 CD ARG 7		.708 44.582	1.000 12.85
ATOM 590	NE ARG 7		02 1741 .685 43.347	237 62 - 15
ANISOU 590	NE ARG 7			1.000 13.71 188 90 - 91
ATOM 591	CZ ARG 7	5 -3.984 21	.036 43.013	1.000 12.46
ANISOU 591	CZ ARG 7	_		-89 86 1 1 7
ATOM 592 ANISOU 592	NH1 ARG 7 NH1 ARG 7		.241 43.894	1.000 14.64
ATOM 593	NH2 ARG 7		94 1834 .167 41.794	186 -91 6 5 1.000 13.72
ANISOU 593	NH2 ARG 7			-136 84 - 83
ATOM 594	C ARG 7	5 [-7.948 20]	.787 48.475	1.000 12.74
ANISOU 594 ATOM 595	C ARG 7			-209 214 -464
ANISOU 595	O ARG 7 O ARG 7		.944 48.818	1.000 14.60
ATOM 596	N GLY 7		26 2273 .955 49.078	-427 156 $-480$ 1.000 11.92
ANISOU 596	N GLY 7		<del>-</del>	-22 34 - 389
ATOM 597	CA GLY 7	6 -8.801 22	.395 50.070	1.000 12.44
ANISOU 597 ATOM 598	CA GLY 7			-315 263 -412
ANISOU 598	C GLY 7 C GLY 7		.857 51.469	1.000 12.50
ATOM 599	0 GLY 7		27 1900 .517 51.769	5 326 - 273 1.000 14.25
ANISOU 599	O GLY 7			-277 239 - 225
ATOM 600	N PHE 7		.840 52.287	1.000 12.65
ANISOU 600 ATOM 601	N PHE 7 CA PHE 7		·	-162 231 -351
ANISOU 601	CA PHE 7		.474 53.694 10 1914	1.000 14.00
ATOM 602	CB PHE 7		.226 54.451	-260 276 $-138$ 1.000 14.73
ANISOU 602	CB PHE 7		· · · · ·	-402 485 -317
ATOM 603 ANISOU 603	CG PHE 7	_	.824 55.912	1.000 17.13
ATOM 604	CG PHE 7 CD1 PHE 7	, ,		-374 378 $-243$
ANISOU 604	CD1 PHE 7		.369 56.886 00 1962	1.000 19.49 -119 219 -789
ATOM 605	CD2 PHE 7			1.000 19.13
ANISOU 605	CD2 PHE 7	7 2348 30	68 1852	-501 864 -165
ATOM 606 ANISOU 606	CE1 PHE 7	_		1.000 19.75
ATOM 607	CE1 PHE 7 CE2 PHE 7		81 2168	-174 -313 -304
ANISOU 607	CE2 PHE 7			1.000 18.73 -382 310 - 77
ATOM 608	CZ PHE 7			1.000 19.22
ANISOU 608	CZ PHE 7	7 2378 25	42 2382	98 13 - 364
ATOM 609 ANISOU 609	C PHE 7 C PHE 7	_	.976 53.924	1.000 13.73
ATOM 610		7 1306 20 7 -10.520 19		-368 21 - 204 1 000 16 02
ANISOU 610		7 1386 25		$1.000 \cdot 16.02$ $-470  -128  -425$
			- 4474	1.0 120 - 423

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						- 110 -		
ATOM	611	N	THR	78	-8.869	19.439	54.852	1.000 14.33
ANISOU	611	N	THR	78	1543	2270	1629	-472 35 - 49
ATOM	612	CA	THR	78	-9.034	18.053	55.276	1.000 15.80
ANISOU	612	CA	THR	78	1813	2310	1880	-508 -23 8 2
ATOM	613	CB	THR	78	-8.001	17.081		
ANISOU	613	CB	THR				54.666	1.000 18.26
				78	1583	2199	3158	-599 334 131
ATOM	614	0G1	THR	78	-7.924	17.323	53.266	1.000 21.81
ANISOU	614	0G1	THR	78	3351	1877	3057	-88 943 -370
ATOM	615	CG2		78	-8.419	15.634	54.888	1.000 20.35
ANISOU	615	CG2	THR	78	2855	2254	2622	-1119 1108 - 707
ATOM	616	С	THR	78	-8.832	17.881	56.777	1.000 19.14
ANISOU	616	C	THR	78	2845	2479	1948	-1747 -471 1 6 9
ATOM	617	0	THR	78	-7.801	18.311	57.290	1.000 22.04
ANISOU	617	0	THR	78	2781	2889	2704	-1718 -985 7 6 3
ATOM	618	N	GLY	79	-9.730	17.203	57.484	1.000 19.20
ANISOU	618	N	GLY	79	2629	2823	1844	-1352 19 4 5
ATOM	619	CA	GLY	79	-9.429	16.695	58.819	1.000 16.69
ANISOU	619	CA	GLY	79	1800	2770	1771	-518 196 - 95
ATOM	620	С	GLY	79	-8.672	15.376	58.720	1.000 22.98
ANISOU	620	С	GLY	79	2381	2874	3477	-272 -289 - 545
ATOM	621	0	GLY	79	-9.227	14.504	58.044	1.000 25.57
ANISOU	621	Ō	GLY	79	3683	2520 .	3514	-456 -974 - 141
ATOM	622	N	LEU	80	-7.494	15.236	59.319	1.000 22.91
ANISOU	622	N	LEU	80	2412	2900	3392	
ATOM	623	CA	LEU	80	-6.644	14.081	59.072	
ANISOU	623	CA	LEU	80	2848	2777		1.000 25.08
ATOM	624	C	LEU	80			3904	206 621 361
ANISOU	624	C	LEU		-6.372	13.294	60.370	1.000 24.30
ATOM	625	0		-	2834	2762	3637	-300 480 200
ANISOU	625	0	LEU	80	-5.729	13.812		1.000 25.14
ATOM	626	_	LEU	80	2253	3017	4283	27 145 - 5
ANISOU	626	CB	LEU	0.8	-5.318	14.480	58.415	
		CB	LEU	80	3057	3326	3937	379 918 641
ATOM	627	CG	LEU	80	-4.411		57.933	
ANISOU	627	CG	LEU	80	3474	3505	4204	287 1260 1 7 3
ATOM	628	CD1	LEU	80	-5.145		56.956	
ANISOU	628		LEU	8 0	5673	3891	4993	-1554 1987 - 287
ATOM	629		LEU	80	-3.137		57.306	
ANISOU	629		LEU	8 0	3502	3919	3920	125 1307 - 264
ATOM	630	N	GLU	81	-6.853	12.055	60.396	1.000 25.58
ANISOU	630	N	GLU	81	2469	2759	4490	-196 -82 510
ATOM	631	CA	GLU	81	-6.739	11.038	61.415	1.000 25.98
ANISOU	631	CA	GLU	81	2739	2692	4441	-258 -55 424
ATOM	632	C	GLU	81	-5.299	10.536	61.562	1.000 26.28
ANISOU	632	С	GLU	81	2870	3268	3848	187 407 841
ATOM	633	0	GLU	81	-4.489	10.655	60.655	1.000 28.19
ANISOU	633	0	GLU	81	3709	3520	3483	253 799 - 544
ATOM	634	CB	GLU	81	-7.685	9.861	61.123	1.000 29.83
ANISOU	634	CB	GLU	81	3533	2894		-770 270 181
ATOM	635	CG	GLU	81	-7.241	8.832	60.098	
ANISOU	635	CG	GLU	81	1737	2915	4976	284 -1220 1 5 8
ATOM	636	CD	GLU	81	-7.568	9.156	58.649	
ANISOU	636	CD	GLU	81	1841	3405	5012	475 -1887 - 456
ATOM	637		GLU	81	-8.120	10.240	58.324	1.000 28.81
ANISOU	637		GLU	81	3444	3091	4413	322 -155 7 9 1
ATOM	638		GLU	81	-7.240	8.273	57.814	1.000 31.31
ANISOU			GLU	81	3514	3384	4999	162 352 100
ATOM	639	N	SER	82	-4.988	9.974	62.720	1.000 31.00
ANISOU		N	SER	82	3568	3780	4430	-65 -30 1484
ATOM	640	CA	SER	82	-3.653	9.422	62.959	
ANISOU		CA	SER	82	3692			
ATOM	641	CA				3278	4540	-157 -515 1011
111 011	0 4 7		SER	82	-3.421	8.150	62.150	1.000 31.76

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- 111 -ANISOU 641 SER 82 3995 3241 -102 -1104 8 4 7 4831 ATOM 642 0 SER 82 -4.3137.728 61.397 1.000 34.01 ANISOU 642 82 0 SER 3193 5935 -1188 1 3 4 3794 458 ATOM 643 SER CB 82 9.167 -3.463 64.452 1.000 34.74 ANISOU 643 SER CB 82 4687 3907 -232 -979 9 7 1 4606 ATOM 644 SER 0G 82 -2.3608.305 64.681 1.000 41.53 ANISOU 644 OG 82 SER 4922 5366 5490 236 -1958 970ATOM 645 -17.230 9.498 GLY Ν 91 70.136 1.000 42.64 ANISOU 645 Ň GLY 91 4516 7599 -2166 2340 - 427 4086 ATOM 646 -17.485 10.892 CAGLY 91 69.789 1.000 44.91 ANISOU 646 CAGLY 91 6666 7702 2697 -4311 -1561 565 ATOM 647 C GLY -16.227 11.662 91 69.452 1.000 38.67 ANISOU 647 GLY Ç 5455 91 7587 1652 -2821 -274 - 159 ATOM 648 -15.164 11.480 0 GLY 91 70.040 1.000 32.45 ANISOU 648 GLY 0 91 4241 4474 3616 -183 1152 - 439 ATOM 649 N GLY -16.332 12.558 92 68.474 1.000 31.97 ANISOU 649 GLY N 92 3881 5904 2363 -1382 735 - 571 ATOM 650 CA-15.232 13.412 GLY 92 68.075 1.000 33.02 ANISOU 650 CAGLY 92 4121 6150 2274 -1716 851 - 956 ATOM 651 C GLY 92 -15.223 13.696 66.572 1.000 26.22 ANISOU 651 C GLY 92 2603 5046 2314 -885 741 - 947 ATOM 652 0 GLY -16.289 13.666 92 65.939 1.000 23.91 ANISOU 652 0 92 GLY 2490 3396 3198 -680 - 5 6 7 548 653 ATOM N SER -14.010 13.956 93 66.088 1.000 23.77 ANISOU 653 Ν SER 93 2405 3917 2708 -372 736 - 560 ATOM 654 SER -13.801 14.287 CA 93 64.690 1.000 23.41 ANISOU 654 CA SER 93 2700 3292 2901 -386 970 MOTA 655 C SER -12.410 13.852 93 64.240 1.000 24.26 ANISOU 655 C SER 93 <sup>2</sup>2547 3908 2763 -286 833 - 224 656 ATOM 93 -11.497 13.831 0 SER 65.089 1.000 27.06 ANISOU 656 SER 0 93 3536 3401 3346 630 92 - 386 ATOM 657 SER -13.966 15.795 CB 93 64.467 1.000 25.71 ANISOU 657 CB SER 93 2811 3225 3735 -576 271 - 506 ATOM 658 OG -13.558 16.158 SER 93 63.150 1.000 28.14 ANISOU 658 OG SER 93 2694 3713 4284 -373 290 517 ATOM 659 N -12.254 13.533 TYR 94 62.949 1.000 24.24 ANISOU 659 TYR N 94 2786 3320 3104 -204 791 - 8 1 7 ATOM 660 CATYR 94 -10.878 13.262 62.498 1.000 23.94 ANISOU 660 CA TYR 94 3089 2502 3505 95 1112 - 683 ATOM 661 C -10.017 14.531 TYR 94 62.584 1.000 25.19 ANISOU 661 C 94 TYR 2601 2657 4312 147 737 - 625 ATOM 662 -8.786 14.421 62.694 1.000 30.11 TYR 94 ANISOU 662 0 TYR 2617 94 3095 5726 307 760 3 6 663 ATOM -10.800 12.659 CB TYR 94 61.098 1.000 25.64 ANISOU 663 TYR CB 3566 94 2910 3267 -293 1331 - 525 664 MOTA CG TYR -11.600 11.410 94 60.876 1.000 23.22 ANISOU 664 CG TYR 3359 2697 94 2768 -69 784 - 274 ATOM CD1 TYR 665 -12.451 11.455 94 59.777 1.000 26.01 ANISOU 665 CD1 TYR 94 2741 4410 2730 499 353 - 543 ATOM CD2 TYR 666 -11.564 10.252 61.635 1.000 24.42 94 ANISOU 666 CD2 TYR 94 3117 2866 3297 73 458 - 1 4 CE1 TYR ATOM 667 -13.243 10.407 94 59.443 1.000 28.75 ANISOU 667 CE1 TYR 4559 94 3328 3037 140 - 1370 434 CE2 TYR ATOM 668 -12.375 9.159 94 61.305 1.000 26.47 ANISOU 668 CE2 TYR 94 4707 2585 2764 -220 1227 - 718 MOTA 669 CZTYR -13.209 9.247 94 60.212 1.000 29.70 ANISOU 669 CZTYR 94 5641 3518 2125 -1172 1103 - 1447 ATOM 670 OH TYR -14.059 8.281 94 59.730 1.000 34.02 ANISOU 670 OH TYR 94 3079 3962 -423 1593 - 2638 5886 ATOM 671 N SER -10.628 15.714 95 62.561 1.000 22.61 ANISOU 671  $\mathbf{N}$ SER 95 2460 2497 3632 -54 59 - 338

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16.975
ATOM
       672
            CA
                SER
                      95
                          -9.924
                                          62.750 1.000 22.54
                          2257
ANISOU 672
                SER
            CA
                      95
                                  2603
                                          3706
                                                  -120
                                                        -301 4 6
ATOM
       673
            C
                SER
                                  17.106
                      95
                          -9.370
                                          64.163
                                                  1.000 23.58
ANISOU 673
            C
                SER
                                  3478
                      95
                          1811
                                                  -521
                                                        -88 -85
                                          3671
ATOM
       674
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                SER
                      95
                          -8.623
                                  18.034
                                          64.481
                                                  1.000 26.53
ANISOU 674
                SER
            0
                      95
                          2592
                                  3242
                                          4247
                                                        -167 - 641
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ATOM
       675
                SER
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            CB
                      95
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                SER
ANISOU 675
            CB
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                                          4264
                          3657
                                                  365
                                                        -379 2 8
ATOM
       676
                SER
            OG
                      95
                          -11.506 18.093
                                          61.242
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ANISOU 676
                SER
                      95
            0G
                          6336
                                  4214
                                          4421
                                                  900
                                                        -1445 1442
ATOM
       677
                ASP
            N
                      96
                          -9.712
                                  16.194
                                                  1.000 25.04
                                          65.060
                ASP
ANISOU 677
                      96
            N
                          2579
                                  3688
                                                  -399 277 -232
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MOTA
       678
                ASP
            CA
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                          -9.228
                                  16.317
                                          66.422
                                                  1.000 24.42
ANISOU 678
            CA
                ASP
                      96
                          2603
                                  3347
                                                  -470 257 -526
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                                  16.050
ATOM
       679
                ASP
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            C
                          -7.735
                                          66.501
                                                  1.000 24.45
ANISOU 679
            C
                ASP
                      96
                          2597
                                  3228
                                          3466
                                                  -471
                                                        162 - 383
ATOM
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ANISOU 680
            0
                ASP
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                          2656
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ATOM
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            CB
                ASP
                          -9.952
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                                          67.334
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ANISOU 681
                ASP
            CB
                          2310
                      96
                                  3806
                                                  -423
                                                        -228 7 7
                                          3371
            CG
ATOM
       682
                ASP
                      96
                          -11.411 15.605
                                         67.606
                                                  1.000 26.77
ANISOU 682
            CG
                ASP
                          2272
                                          3566
                      96
                                  4334
                                                  -362
                                                        -240716
ATOM
       683
            OD1 ASP
                          -11.935 16.723
                                                  1.000 33.94
                      96
                                          67.388
ANISOU 683
            OD1 ASP
                          3267
                      96
                                  4894
                                          4733
                                                  647
                                                        204 569
ATOM
       684
            OD2 ASP
                          -12.058 14.646
                                                  1.000 32.65
                      96
                                          68.083
            OD2 ASP
ANISOU 684
                      96
                          3624
                                  4709
                                          4072
                                                  -1032 1446 - 202
ATOM
       685
                TYR
                      97
                          -7.254
                                 15.226
            N
                                          65.581
                                                  1.000 22.21
ANISOU 685
            N
                TYR
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                         2292
                                  3389
                                          2760
                                                  -376 -77 -102
                                  14.852
MOTA
       686
            CA
                TYR
                         ^{-}5.835
                      97
                                          65.583
                                                  1.000 23.71
ANISOU 686
            CA
                TYR
                      97
                          2480
                                  3542
                                          2987
                                                  -27
                                                        106 644
ATOM
                          -5.026
       687
            C
                TYR
                      97
                                  15.828
                                          64.743
                                                  1.000 23.06
ANISOU 687
                      97
            C
                TYR
                          2363
                                  3754
                                          2647
                                                  -410
                                                       -78 350
ATOM
       688
                TYR
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                      97
                          -3.992
                                          65.230
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                                  16.327
                          2205
ANISOU 688
                TYR
                      97
                                  3845
                                          3178
                                                  -133 -230 7 4
ATOM
       689
                TYR
            CB
                      97
                          -5.585
                                          65.035
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                                                  1.000 28.38
ANISOU 689
                TYR
            CB
                          3230
                                  3324
                      97
                                          4229
                                                  540
                                                        -450 8 3 2
                TYR
MOTA
       690
            CG
                      97
                          -4.132
                                  13.025
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ANISOU 690
            CG
                TYR
                                          4161
                          3278
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                                  4101
                                                  766
                                                        -191 6 7 1
                         -3.511
ATOM
            CD1 TYR
       691
                      97
                                 12.691 66.285
                                                  1.000 30.19
ANISOU 691
            CD1 TYR
                          2878
                      97
                                  4475
                                          4119
                                                  1106 151 951
                      97 -3.370 12.945 63.922 1.000 29.79
ATOM 692
            CD2 TYR
ANISOU 692
           CD2 TYR
                     97
                          3317
                                          3997
                                  4005
                                                  53 - 253 544
ATOM
       693 CE1 TYR
                          -2.178 12.294 66.324 1.000 32.77
                     97
ANISOU 693
            CE1 TYR
                                          5126
                     97
                          2554
                                  4771
                                                  574
                                                        -68 763
ATOM
       694
            CE2 TYR
                                 12.553 63.955 1.000 32.68
                     97
                          -2.043
ANISOU 694
            CE2 TYR
                      97
                          3536
                                  3793
                                          5087
                                                  403
                                                        353 323
MOTA
                          -1.445
       695
            CZ
                TYR
                                                  1.000 33.00
                      97
                                  12.228 65.157
ANISOU 695
             CZ
                TYR
                      97
                          2633
                                  4284
                                          5622
                                                  1066 264 456
ATOM
       696
                TYR
                                  11.845 65.156 1.000 42.66
             OH
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                      97
ANISOU 696
                TYR
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             OH
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                                          8264
                                                  1161 764 1277
                      97
ATOM
       697
             CB
                 SER
                                  16.575 62.134 1.000 23.20
                      98
                          -3.465
ANISOU 697
             CB
                 SER
                      98
                                  2766
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       698
ATOM
                 SER
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             OG
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                          -3.632
ANISOU 698
                 SER
                      98
             OG
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ATOM
        699
             C
                 SER
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                          -5.694
                                  17.744 61.701 1.000 18.66
ANISOU 699
             C
                 SER
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ATOM
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                 SER
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ANISOU 700
                 SER
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                      98
                                          2646
                                                  -945 -249 1 8 1
ATOM
       701
                 SER
                     98
             N
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ANISOU 701
                                                  -441 -395 6 0 5
             N
                 SER
                          2816
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                                  3227
                                          2931
ATOM · 702
                 SER 98
             CA
                          -4.748 17.143 62.741 1.000 21.31
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- 113 -ANISOU 702 CASER 98 2687 2430 2982 153 294 133 703 ATOM MET N -5.30718.891 99 1.000 18.68 61.148 ANISOU 703 N MET 99 2392 2722 1984 -978 -366 1 0 1 ATOM 704 CAMET 99 -6.04719.560 60.075 1.000 17.84 ANISOU 704 2431 CAMET 99 2620 1726 -945 -212 - 17705 ATOM CB MET -6.819 20.779 99 1.000 19.71 60.585 ANISOU 705 CB 99 MET 2348 2173 2968 -679 25 6 4 ATOM 706 MET CG 99 -8.052 20.392 61.374 1.000 23.68 ANISOU 706 CG MET 99 3582 2360 3055 393 489 -504 707 ATOM MET SD 99 -9.031 21.821 61.911 1.000 22.33 ANISOU 707 2569 SD MET 99 3383 2534 -522 170 - 120 708 ATOM CE 99 MET -8.14822.225 63.419 1.000 36.98 ANISOU 708 CE MET 99 6485 4165 3401 -225 -1904 - 23709 MOTA С MET -5.07099 58.973 19.954 1.000 17.19 ANISOU 709 C MET 2269 99 2488 .1776 -960 -194 - 201710 ATOM 0 -3.964 MET 99 20.341 59.324 1.000 16.93 ANISOU 710 MET 0 1932 99 2583 1919 -367 -208 - 241100 -5.486 ATOM 711 CYS N 19.864 57.715 1.000 20.00 ANISOU 711 N CYS 100 3178 2683 1739 -1753 -358 1 6 6 ATOM 712 100 -4.645 CACYS 56.554 1.000 16.64 20.181 ANISOU 712 CA CYS 100 2213 2294 1817 -924 -563 4 6 8 713 ATOM CB CYS 100 - 4.29118.893 55.813 1.000 17.74 ANISOU 713 CBCYS 2174 100 2161 2407 -765 1053 560 ATOM 714 SG CYS 100 -3.035 18.928 54.552 1.000 33.56 ANISOU 714 SG CYS 100 5244 3511 3997 414 1509 6 0 1 MOTA 715 CYS C 100 - 5.34721.121 55.590 1.000 13.48 ANISOU 715 C CYS 1415 100 1879 1829 -68 240 - 91ATOM 716 CYS 0 100 - 6.58521.127 55.496 1.000 14.49 ANISOU 716 0 CYS 100 1880 1952 1673 -497 -57 1 4 717 ATOM 21.921 N TYR 101 - 4.58954.852 1.000 13.35 ANISOU 717 TYR N101 1721 1677 1673 -254 - 78ATOM 718 CATYR 101 -5.016 53.755 1.000 10.27 22.753 ANISOU 718 CA 101 926 1498 TYR 1477 -15 -141 - 231ATOM 719 CB TYR 101 -5.102 24.265 54.124 1.000 13.60 ANISOU 719 CBTYR 101 1626 1513 2027 -48 322 ATOM 720 CG 101 -5.498 TYR 25.025 52.863 1.000 17.31 ANISOU 720 TYR CG 101 2373 1509 2694 -158 -103 1 9 3 CD1 TYR ATOM 721 101 -6.815 25.068 52.519 1.000 16.38 ANISOU 721 CD1 TYR 101 2464 752 3006 190 -227722 ATOM CE1 TYR 25.715 51.412 1.000 17.01 101 - 7.307ANISOU 722 CE1 TYR 101 2755 714 2993 -86 -416 723 MOTA CD2 TYR 25.679 52.012 1.000 19.51 101 -4.616 ANISOU 723 CD2 TYR 101 3032 1533 2847 -1143 -594 4 7 5 ATOM CE2 TYR 724 101 -5.065 26.321 50.872 1.000 20.96 ANISOU 724 CE2 TYR 101 2802 1949 3211 238 112 769 ATOM 725 CZTYR 26.334 50.568 1.000 22.78 101 -6.414 ANISOU 725 101 3238 CZTYR 2291 -1228 -919 6 2 4 3126 MOTA 726 OH TYR 26.986 49.442 1.000 23.10 101 - 6.875ANISOU 726 OH 101 3141 TYR 3112 2522 -129 4 2 9 -14 ATOM 727 C TYR 22.518 52.596 1.000 11.25 101 -4.041 ANISOU 727 C TYR 101 1223 1398 -323 103 -252 1654 MOTA 728 0 TYR 101 -2.823 22.677 52.787 1.000 12.23 ANISOU 728 0 TYR 101 1114 1750 1784 -87 130 - 20 729 ATOM N SER 102 -4.542 22.190 51.405 1.000 11.17 ANISOU 729 N SER 102 1355 1611 1279 -220 145 - 263102 -3.752 ATOM 730 CASER 21.802 .50.235 1.000 10.46 ANISOU 730 102 1144 CASER 1263 1568 62 -1 -125 ATOM 731 CB SER 102 - 4.02720.343 49.908 1.000 13.46 ANISOU 731 CB SER 102 1668 1212 2234 105 - 301 324 ATOM 732 OG SER 102 -3.723 19.487 51.025 1.000 16.42 ANISOU 732 102 2291 OG SER 1313 2637 -122 -43 9 6

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ATOM 733 C SER 22.668 102 - 4.04649.008 1.000 11.74 C ANISOU 733 SER 102 1346 1500 1614 18 - 39 - 10 ATOM 734 0 SER 102 -5.148 23.148 48.784 1.000 12.84 ANISOU 734 102 1480 0 SER 1988 90 -66 2 4 9 1410 ATOM 735 MET 103 -3.004 22.871 48.187 1.000 12.33 Ν 103 1554 ANISOU 735 N MET 1409 1722 -262 -10 -246 103 -3.188 736 ATOM CAMET 23.603 46.938 1.000 12.92 103 1663 ANISOU 736 CAMET 1681 1565 22 47 - 70 CB ATOM 737 MET 103 -3.215 25.122 47.179 1.000 17.51 ANISOU 737 1634 CB MET 103 2439 2579 -363 812 -.44 103 -1.929 CG ATOM 738 MET-25.808 47.549 1.000 20.07 ANISOU 738 CG MET 103 2509 1470 3646 -538 688 376 103 -2.136 739 SD ATOM MET 27.614 1.000 18.10 47.689 ANISOU 739 103 2235 SD MET 1665 2975 -3 - 334 - 352103 -2.365 MET 28.068 ATOM 740 CE 45.991 1.000 18.09 ANISOU 740 CE 103 2319 MET 1457 3098 -187 -718 -214MET MOTA 741 C 103 -2.152 23.221 45.892 1.000 12.57 ANISOU 741  $\mathsf{C}$ MET 103 1420 1837 1519 119 ~53 2 3 8 ATOM 742 0 MET 103 -1.120 22.573 46.175 1.000 12.57 103 1094 ANISOU 742 0 -155 -165 2 7 6 MET 1891 1792 GLY ATOM 743 N 104 - 2.41823.650 1.000 12.83 44.655 ANISOU 743 N 104 1493 GLY 1958 1422 237 -124 - 34GLY 1.000 12.65 ATOM 744 23.459 43.513 CA104 - 1.533ANISOU 744 GLY CA104 1075 2188 1544 -93 -37 242 ATOM 745 C GLY 104 - 1.62424.622 42.542 1.000 14.36 104 1909 ANISOU 745 C GLY 1985 1561 -265 -294 1 4 2 GLY 1.000 15.69 ATOM 746 104 -2.033 0 25.700 42.967 ANISOU 746 0 GLY 104 1628 2273 2060 163 -197213ATOM 747 THR N 105~-1.242 24.397 41.276 1.000 14.52 ANISOU 747  $\mathbf{N}$ THR 105 1829 2182 1504 -59 -375 3 1 9 MOTA 748 CA THR 105 -1.218 25.452 40.279 1.000 15.27 ANISOU 748 CATHR 105 1977 2223 1603 -363 3 6 5 -105 MOTA 749 CB THR 105 -0.359 25.083 39.039 1.000 15.61 CB ANISOU 749 THR 2122 1873 -37 105 1936 -106 5 5 4 750 OG1 THR 23.876 MOTA 105 - 0.88438.446 1.000 16.16 ANISOU 750 OG1 THR 105 1738 2260. 2140 217 -285 1 5 1 CG2 THR ATOM 751 105 1.092 24.882 39.369 1.000 17.47 ANISOU 751 CG2 THR 105 1918 2871 1847 -293 -227527752 25.828 ATOM C 105 -2.603 THR 39.755 1.000 14.73 ANISOU 752  $\mathsf{C}$ THR 105 1989 1694 1913 122 -340 1 9 9 753 ATOM 0 THR 105 -2.730 26.921 39.174 1.000 19.91 23 -437 1004 ANISOU 753 THR 105 2579 0 2355 2632 ATOM 754 Ν ALA 106 -3.587 24.960 39.913 1.000 16.57 ANISOU 754 ALA 106 1836 N 2413 2047 2 -260 661 755 ATOM ALA 1.000 14.94 106 - 4.97525.167 39.465 CA ANISOU 755 ALA CA-456 3 6 5 106 1975 1904 1798 105 ATOM 756 CB ALA 106 -5.054 24.945 37.965 1.000 17.75 ANISOU 756 CB ALA 2862 1876 140 -201 - 32106 2006 757 ATOM C 106 -5.942 ALA 24.251 40.222 1.000 16.26 ANISOU 757 ALA C 106 1710 2174 2293 327 -127491ATOM 758 ALA 0 106 -5.498 1.000 14.57 23.398 41.013 ANISOU 758 ALA 106 1622 1971 -21 3 3 7 0 1945 213 40.008 1.000 16.71 ATOM 759 N 107 - 7.253ASP 24.410 107 1768 ANISOU 759 ASP 540 -22 304 N2096 2485 ATOM 760 ASP 40.633 1.000 16.10 CA107 - 8.31023.638 ANISOU 760 CAASP 107 1696 2175 2246 51 - 485 - 14761 ATOM CB ASP 107 -8.231 22.171 40.211 1.000 17.09 ANISOU 761 ASP CB 107 1299 2385 2808 -203 - 399144 ATOM 762 CG ASP 107 - 8.41821.966 38.720 1.000 21.54 ANISOU 762 CG ASP 2894 2906 84 - 317 - 722 107 2385 ATOM 763 OD1 ASP 22.445 38.189 1.000 23.92 107 -9.452

		145	
OD1 ASP OD2 ASP OD2 ASP OD0 ASS OD1 AS	108 1861 109 -9.412 109 1458 109 -10.602 109 1094 109 -11.187 109 -11.580 109 -11.931 109 -11.931 109 -12.780 109 -12.780 109 -10.203 109 -10.203 109 -10.203 109 -9.416 109 -9.416 110 -10.298 110 1626 110 -9.660 110 1423 110 -8.425 110 -8.425 110 1702 110 -7.257 110 1885 110 -8.405 110 -6.102 110 1958 110 -7.288	4004       2954         23.785       42.160         1918       2201         22.850       42.936         1927       2390         25.020       42.598         1866       1870         25.314       44.031         1823       1898         26.420       23.09         25.942       43.963         2141       2142         24.932       44.505         1998       43.094         26.678       43.094         25.708       44.642         1937       2120         23.36       2219         25.796       46.769         1923       47.331         1959       23.383         1648       1994         25.796       46.769         1923       47.331         25.796       46.769         1959       23.383         1674       23.783         23.783       47.089         26.794       47.840         1989       47.786         2042       47.786	105
CD1 PHE CD2 PHE CD2 PHE CE1 PHE CE1 PHE CE2 PHE CE2 PHE CZ PHE CZ PHE CZ PHE C PHE C PHE C PHE	110 1885 110 -8.405 110 2073 110 -6.102 110 1958 110 -7.288 110 2158 110 -6.118 110 1925 110 -11.495 110 1774 110 -12.562	2462 3387 30.110 45.789 2226 3419 29.347 47.065 2116 3332 29.846 45.050 2094 3596 29.496 45.694 2131 3327 29.556 49.538 1806 2911	461 573 - 707 1.000 20.31 512 712 - 264 1.000 19.49
	ASPPPNNNNNNNNNNNNNNNNUUUUUUUUUUUUUUUUUUU	OD2 ASP 107 -7.563 OD2 ASP 107 2496 C ASP 107 1261 O ASP 107 -8.507 O ASP 107 2017 N ASN 108 -8.027 N ASN 108 2093 CA ASN 108 27.967 CA ASN 108 27.967 CA ASN 108 27.967 CA ASN 108 1593 CG ASN 108 1593 CG ASN 108 1593 CG ASN 108 1505 OD1 ASN 108 25.516 CG ASN 108 25.516 CG ASN 108 25.516 CG ASN 108 25.086 OD1 ASN 108 25.086 OD1 ASN 108 25.086 OD1 ASN 108 215.086 OD1 ASN 108 25.086 OD2 ASN 108 25.086 OD3 ASN 108 25.086 OD4 ASN 108 25.086 OD5 ASN 108 25.086 OD6 ASN 108 25.086 OD7 ASN 108 25.086 OD7 ASN 108 25.086 OD8 25.086 OD9 25.	OD1

ATOM 794 111 -11.406 29.717 50.851 1.000 19.41 PRO NANISOU 794 PRO N 2110 111 2279 2985 -386 519 -314 ATOM 795 PRO 111 -10.278 29.322 51.705 1.000 19.20 CD CD PRO ANISOU 795 1880 2640 -417 255 -514 111 2773 111 -12.549 30.252 51.604 1.000 21.47 ATOM 796 PRO CAANISOU 796 CAPRO 1924 111 3026 3206 -50 728 - 635CB PRO 111 -12.167 30.007 ATOM 797 53.055 1.000 23.63 ANISOU 797 CB PRO 2054 111 3789 3137 334 776 - 575 ATOM CG 111 -10.775 29.535 53.100 1.000 22.33 798 PRO ANISOU 798 PRO CG 111 2767 2908 2809 -1006 623 -414 111 -12.828 31.739 51.433 1.000 23.88 799 PRO ATOM C ANISOU 799 C PRO 111 3139 79 -142 - 479 2049 3887 800 PRO 111 -13.919 32.194 51.834 1.000 26.77 ATOM 0 ANISOU 800 PRO 0 111 3800 2818 3555 992 -91 - 397801 N SER 112 -11.906 32.517 50.872 1.000 25.19 ATOM ANISOU 801 SER 112 3514 2269  $\mathbf{N}$ 3788 -247 -856 2 8 2 112 -12.300 33.919 50.631 1.000 26.43 ATOM 802 SER CAANISOU 802 CASER 2655 4734 112 2654 496 1364 4 5 6 ATOM 803 CB SER 112 -12.506 34.712 51.912 1.000 33.37 ANISOU 803 CB SER 112 3122 3663 5895 2582 - 510172 MOTA 804 OG SER 112 -11.322 34.719 52.688 1.000 36.94 112 6530 ANISOU 804 OG SER 2154 5351 1399 206 -415 805 112 -11.262 34.587 49.723 1.000 26.62 ATOM  $\mathsf{C}$ SER ANISOU 805 SER C 112 2613 2546 4956 1021 1668 6 5 1 ATOM 112 -10.219 34.029 49.414 1.000 22.81 SER 806 0 ANISOU 806 SER 0 112 2241 2782 3645 800 837 - 400ATOM 807 GLY 113 -11.570 35.802 49.279 1.000 28.93  $\mathbf{N}$ ANISOU 807 NGLY 113 2937 2947 5108 1008 1175 1198 CA GLY ATOM 808 113 -10.659 36.478 48.365 1.000 30.79 ANISOU 808 GLY CA113 2992 3606 5102 381 798 1400 809 ATOM GLY 113 -9.362 C 36.829 49.070 1.000 31.83 ANISOU 809 C GLY 113 3297 3919 4878 262 897 528 GLY 36.790 ATOM 810 113 -8.294 0 48.459 1.000 25.85 ANISOU 810 GLY 113 2920 0 4585 857 2317 450 - 203114 -9.479 ATOM 811 ASP 50.365 1.000 29.56 N 37.145 ANISOU 811 ASP 866 N 114 3487 2877. 4868 1104 7 6 0 MOTA 812 ASP 114 -8.257 CA 37.463 51.122 1.000 26.15 ANISOU 812 114 3189 CAASP 2680 4066 1028 1584 5 4 2 ATOM 813 CB ASP 114 -8.628 37.937 52.526 1.000 33.81 ANISOU 813 CB ASP 2697 4569 114 5580 1774 1691 - 240 ATOM 814 CG ASP 114 -7.904 39.232 52.840 1.000 40.77 CG ASP ANISOU 814 114 6798 719 693 - 248 3734 4960 OD1 ASP 114 -8.330 40.277 52.295 1.000 48.61 ATOM 815 OD1 ASP 114 6014 2534 ANISOU 815 9920 1703 931 -913 OD2 ASP ATOM 816 114 -6.932 39.178 53.622 1.000 54.35 OD2 ASP 114 5258 ANISOU 816 7609 7783 -868 495 1602 817 ATOM ASP 114 -7.310 36.281 51.231 1.000 23.05 C 114 2621 ANISOU 817 ASP C 2102 4033 1874 3 4 0 444 ATOM 818 ASP 114 -6.111 36.371 50.955 1.000 22.05 0 ANISOU 818 ASP 114 2423 2277 3677 131 1411 - 461 ATOM 819 PHE  $\mathbf{N}$ 115 -7.854 35.160 51.637 1.000 23.21 ANISOU 819 115 2945 PHE N 1890 3984 -130 1293 - 228 ATOM PHE 820 115 -7.120 33.896 51.690 1.000 19.93 CAANISOU 820 115 2562 PHE CA3102 -198 655 -294 1908 ATOM 115 -8.085 32.792 52.157 1.000 19.49 821 PHE CB ANISOU 821 PHE 1754 CB 115 2378 3275 64 881 - 314 ATOM 115 -7.523 31.445 52.540 1.000 17.25 822 CG PHE ANISOU 822 CG PHE 115 2053 1589 2912 -56 348 -695 ATOM 823 CD1 PHE 115 -7.637 30.951 53.833 1.000 19.00 CD1 PHE 115 2728 1539 2950 73 496 - 683 ANISOU 823 CD2 PHE 115 -6.868 30.634 51.615 1.000 17.88 ATOM 824

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<del>-</del> 117 -ANISOU 824 CD2 PHE 115 1933 1931 2927 7 298 -810 ATOM 825 CE1 PHE 115 -7.100 29.711 54.163 1.000 20.25 ANISOU 825 CE1 PHE 115 2825 1825 3042 317 341 - 575 826 ATOM CE2 PHE 115 -6.338 29.412 1.000 19.11 51.955 ANISOU 826 CE2 PHE 115 1865 2158 3237 336 351 ATOM 827 CZPHE 115 -6.452 28.936 53.233 1.000 19.39 ANISOU 827 CZPHE 115 2068 1910 3390 320 248 -669 828 ATOM C PHE 115 -6.506 33.624 50.327 1.000 17.86 ANISOU 828 C PHE 115 1964 1945 61 344 1 6 2878 ATOM 829 0 33.315 PHE 115 -5.324 50.271 1.000 17.34 ANISOU 829 0 PHE 115 1868 2107 2613 -132 179 157 830 ATOM N GLU 116 -7.310 33.683 49.263 1.000 18.21 ANISOU 830 NGLU 116 1921 1934 3065 547 281 MOTA 831 CAGLU 116 -6.848 33.387 47.907 1.000 19.99 ANISOU 831 CA 116 2128 GLU 2618 2851 81 231 2 2 2 ATOM 832 CB 116 -7.968 GLU 33.605 46.884 1.000 18.61 116 2058 ANISOU 832 CB GLU 1952 3060 231 244 270 MOTA 833 CG 116 -7.398 GLU 33.378 45.482 1.000 18.61 ANISOU 833 CG 116 1813 GLU 2288 295 2971 -32 - 33ATOM 834 CDGLU 116 -8.442 33.230 44.412 1.000 22.40 ANISOU 834 CDGLU 116 1908 3193 3410 -122 -278 - 91OE1 GLU ATOM 835 116 - 9.65433.272 1.000 30.82 44.678 OE1 GLU ANISOU 835 116 1793 5452 4465 273 -414 - 24836 ATOM OE2 GLU 116 -8.085 33.063 43.225 1.000 30.24 OE2 GLU ANISOU 836 116 3333 5132 3026 382 -658 3 2 7 ATOM 837 C GLU 116 - 5.62034.211 47.535 1.000 18.82 ANISOU 837 C GLU 2990 116 2090 2069 119 487 294 ATOM 838 0 GLU 116, -4.605 33.701 47.049 1.000 17.41 ANISOU 838 0 GLU 116 2228 1780 2606 45 259 282 ATOM 839 **ARG** 35.508 N 117 -5.660 47.777 1.000 21.02 ANISOU 839 117 2313 N ARG 2185 3487 408 220 9 0 ATOM 840 **ARG** CA 117 - 4.56047.431 1.000 21.35 36.420 CA ANISOU 840 ARG 117 2337 1800 3976 466 147 - 31ATOM 841 C ARG 117 - 3.29136.054 1.000 20.52 48.192 ANISOU 841 C **ARG** 117 2292 2124 3380 353 288 - 10MOTA 842 ARG 0 117 - 2.18635.969 47.636 1.000 18.96 ANISOU 842 ARG 0 117 2223 1664 3316 138 318 231 ATOM 843 CB 117 -4:971 ARG 1.000 25.59 37.885 47.693 ANISOU 843 ARG 117 3237 CB 1900 4587 929 1882 6 3 2 ATOM 844 CG ARG 117 -3.881 38.908 47.478 1.000 32.57 ANISOU 844 CG ARG 117 5212 -281 1925 5237 1083 6 2 3 ATOM 845 CD ARG 117 -4.325 40.323 47.859 1.000 36.56 ANISOU 845 CD ARG 117 6009 2157 5724 149 1774 6 6 3 ATOM 846 NEARG 117 -5.162 40.335 49.056 1.000 44.43 ANISOU 846 NE ARG 117 7200 3742 5940 -96 2344 - 15ATOM 847 CZARG 117 - 4.76340.501 50.306 1.000 45.48 ANISOU 847 CZARG 117 6422 4804 6054 -370 2388 - 283 ATOM 848 117 -3.484 NH1 ARG 50.619 1.000 53.21 40.683 ANISOU 848 117 6867 NH1 ARG 6451 6900 -2543 2487 3 5 4 NH2 ARG ATOM 849 117 -5.647 51.301 1.000 50.00 40.487 ANISOU 849 NH2 ARG 117 6265 6511 6220 224 2433 - 1534 850 ATOM 118 -3.439 N ILE 35.832 49.493 1.000 19.30 ANISOU 850 N ILE 118 2275 3221 128 1838 407 - 645 MOTA 851 ILE CA118 - 2.27550.331 1.000 18.25 35.527 ANISOU 851 ILE CA118 2376 78 530 - 449 1745 2811 ATOM · 852 CB ILE 118 -2.665 35.597 51.820 1.000 18.24 ANISOU 852 118 2201 CB ILE 1726 3003 346 906 - 306 ATOM 853 CG2 ILE 34.851 52.732 1.000 18.49 118 - 1.712ANISOU 853 118 2077 CG2 ILE 2158 2792 -202 308 -530 CG1 ILE 118 -2.877 ATOM 854 37.031 52.368 1.000 24.69 ANISOU 854 CG1 ILE 118 4436 3136 1808 284 1382 - 414

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118 -3.786
ATOM
       855
            CD1 ILE
                                37.025
                                        53.582 1.000 29.63
ANISOU 855
            CD1 ILE
                     118 6169
                                 3096
                                         1994
                                                       1258 - 1068
                                                 189
                                 34.172
       856
            C
                     118 -1.692
                                                 1.000 15.65
ATOM
                ILE
                                         49.959
ANISOU 856
                ILE
                                 1549
            C
                     118 2316
                                         2082
                                                 -89
                                                       573 - 117
ATOM
       857
                ILE
                     118 -0.463
                                 34.035
            0
                                         49.802
                                                 1.000 14.59
                     118 2240
ANISOU 857
                ILE
                                 1255
                                         2051
                                                 16 286 2 1 4
                TRP
                     119 -2.523
ATOM
       858
            N
                                 33.139
                                         49.784
                                                 1.000 14.44
ANISOU 858
            N
                TRP
                     119 2125
                                 1592
                                         1771
                                                 47 128 - 71
                TRP
                     119 -2.010
                                 31.795
ATOM
       859
            CA
                                         49.518
                                                 1.000 13.68
ANISOU 859
                TRP
                     119 1712
                                 1529
            CA
                                         1957
                                                 -61
                                                       220 4 0
                                 30.755 49.932
            CВ
                TRP
       860
                     119 -3.089
ATOM
                                                 1.000 14.93
ANISOU 860
            CB
                TRP
                     119 1819
                                 1729
                                         2123
                                                 -234 295 <del>-</del>35
       861
                TRP
                     119 - 2.864
ATOM
            CG
                                 30.482
                                         51.420
                                                 1.000 16.19
                     119 1640
                TRP
                                 2364
ANISOU 861
            CG
                                         2146
                                                 -168
                                                       582 167
       862
            CD2 TRP
ATOM
                     119 -2.116
                                 29.430
                                         51.993
                                                1.000.20.41
ANISOU 862
            CD2 TRP
                     119 3189
                                 2414
                                         2151
                                                 202
                                                       523
                                                           4 0 5
            CE2 TRP
ATOM
       863
                     119 - 2.177
                                 29.580
                                        53.392
                                                1.000 19.84
                                                       234 137
            CE2 TRP
                     119 3536
ANISOU 863
                                                 -439
                                 1818
                                         2184
            CE3 TRP
ATOM
                     119 -1.390
       864
                                 28.357 51.456 1.000 23.94
ANISOU 864
            CE3 TRP
                     119 5382
                                 1647
                                                 561
                                         2068
                                                       126 400
            CD1 TRP
                     119 -3.340
                                         52.460
       865
                                 31.223
ATOM
                                                 1.000 20.05
ANISOU 865
            CD1 TRP
                     119 3207
                                 2343
                                                 -9 189 -139
                                         2069
ATOM
       866
            NE1 TRP
                     119 -2.938
                                 30.689
                                         53.649
                                                 1.000 20.32
                     119 2806
ANISOU 866
            NE1 TRP
                                 2726
                                         2188
                                                 -96
                                                        -68 - 185
                     119 -1.547
            CZ2 TRP
                                                 1.000 22.12
ATOM
       867
                                 28.714
                                         54.281
            CZ2 TRP
                                         2078
ANISOU 867
                     119 4071
                                 2256
                                                       105 2 2
                                                 -17
            CZ3 TRP
ATOM
       868
                     119 -0.761
                                         52.332
                                                 1.000 21.52
                                 27.490
ANISOU 868
            CZ3 TRP
                     119-4214
                                 2168
                                         1794
                                                 311
                                                        -193 1 9 7
       869
            CH2 TRP
ATOM
                     119 -0.847
                                 27.674
                                         53.715
                                                 1.000 24.34
            CH2 TRP
ANISOU 869
                     119 5349
                                                 329
                                 2047
                                         1850
                                                        148 183
                     119 -1.521
                TRP
ATOM
       870
                                 31.634
                                         48.095
                                                 1.000 14.27
            C
                                                 -187 334 - 65
ANISOU 870
            C
                     119 2180
                                 1259
                TRP
                                         1985
                TRP
ATOM
       871
                     119 -0.569
                                 30.865
            0
                                         47.855
                                                 1.000 14.73
ANISOU 871
                TRP
            0
                                 1653
                     119 1996
                                          1946
                                                        362 101
                                                  -67
       872
ATOM
                THR
                     120 - 2.109
                                 32.325
                                         47.116
                                                 1.000 13.99
            N
ANISOU 872
                     120 2231
                                                  106
                                                        627 - 137
            N
                THR
                                 1237
                                          1848
                     120 -1.541
                                         45.762 1.000 15.19
ATOM
       873
                                 32.275
            CA
                THR
ANISOU 873
                THR
                     120 1903
            CA
                                          1774
                                                  9 435 - 242
                                  2093
       874
                THR
                     120 - 2.492
                                 32.983 44.787 1.000 16.41
MOTA
            CB
ANISOU 874
            CB
                THR
                                                  -331 152 6 6
                      120 1934
                                  2304
                                          1995
ATOM 875 OG1 THR 120 -3.738 32.297 44.766 1.000 18.53
            OG1 THR
ANISOU 875
                     120 1891
                                                  -236 195 407
                                  2288
                                          2863
            CG2 THR 120 -1.974 32.906 43.358 1.000 18.02
       876
ATOM
            CG2 THR
ANISOU 876
                     120 2135
                                  2602
                                                  324
                                          2108
                                                        322 3 1 8
MOTA
       877
                THR
                      120 -0.145 32.870 45.727 1.000 14.19
            C
ANISOU 877
                THR
                      120 1868
                                  2050
                                          1475
                                                  87 285 - 167
             C
ATOM
       878
                THR
                      120 0.756
                                  32.299 45.078 1.000 13.62
             0
ANISOU 878
             0
                      120 1864
                                  1692
                                          1620
                                                  301
                                                        354 217
                THR
ATOM
                                  33.962 46.429 1.000 14.55
       879
                GLN
                      121 0.114
            N
ANISOU 879
                      121 1721
             N
                GLN
                                  1672
                                          2136
                                                  304
                                                        175 - 67
                                  34.548 46.483 1.000 15.80
MOTA
       880
             CA GLN
                      121 1.459
ANISOU 880
             CA
                GLN
                                                      -119 3 6 2
                      121 2067
                                  1666
                                          2271
                                                  -18
       881
MOTA
                 GLN
             C
                      121 2.465
                                  33.642 47.176 1.000 13.73
ANISOU 881
             C
                 GLN
                      121 1747
                                  1665
                                          1806
                                                  -30 18 1 1 4
       882
ATOM
                GLN
             0
                      121 3.603
                                  33.452 46.685 1.000 15.36
ANISOU 882
                 GLN
             0
                      121 2063
                                  1688
                                                  48 360 - 4 4
                                          2084
       883
ATOM
             CB GLN
                                  35.918 47.154 1.000 18.85
                      121 1.315
ANISOU 883
             CB
                GLN
                      121 2537
                                  1426
                                          3200
                                                  -73 -5356
             CG GLN
ATOM
       884
                      121 2.639
                                  36.558 47.543 1.000 18.88
                      121 2507 1788
             CG GLN
ANISOU 884
                                          2878
                                                  59 9 - 248
ATOM
       885
             CD GLN
                      121 3.468
                                  36.936 46.337 1.000 20.70
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- 119 -CD GLN ANISOU 885 121 2584 2138 3142 -373 -85 231 886 OE1 GLN ATOM 121 2.935 37.088 45.224 1.000 22.47 OE1 GLN ANISOU 886 121 2695 2822 3019 -245 0 121 ATOM 887 NE2 GLN 121 4.779 37.101 1.000 25.22 46.522 ANISOU 887 NE2 GLN 121 2426 3811 3344 -131 1385 127 888 ATOM TYR N 122 2.081 48.299 33.054 1.000 12.26 ANISOU 888 TYR 1514 N 122 1747 1399 99 - 55 - 258 ATOM 889 Cy TYR 122 2.896 32.102 49.050 1.000 13.18 ANISOU 889 TYR C7 122 1901 1643 1464 -20-253 - 160890 CB ATOM TYR 122 2.211 50.364 31.724 1.000 13.78 ANISOU 890 CB TYR 122 2045 1435 1756 116 48 - 28ATOM 891 CG 122 2.994 TYR 30.808 51.282 1.000 14.22 ANISOU 891 CG 122 1966 TYR 1681 1758 101 68 1 0 1 892 CD1 TYR ATOM 122 4.271 31.120 1.000 17.48 51.722 ANISOU 892 CD1 TYR 122 1788 1972 2882 149 -5 4 2 0 893 ATOM CE1 TYR 122 5.003 52.576 1.000 18.55 30.284 CE1 TYR ANISOU 893 122 2131 2868 2050 102 -404251894 CD2 TYR ATOM 122 2.445 29.619 51.731 1.000 20.72 CD2 TYR 122 3308 ANISOU 894 1366 3197 -519 -1524 3 2 3 CE2 TYR ATOM 895 122 3.140 28.773 52.574 1.000 25.40 CE2 TYR ANISOU 895 122 3772 1812 4067 -782 -2084 8 7 3 896 ATOM TYR 122 4.413 CZ29.101 52.992 1.000 20.93 ANISOU 896 CZTYR 122 2985 1742 3224 -96 -1145 3 1 3 ATOM 897 OH TYR 122 5.068 28.230 53.826 1.000 29.87 ANISOU 897 OH TYR 122 4830 1998 4522 -680 -3078 621 898 ATOM C TYR 122 3.218 30.876 48.209 1.000 12.33 ANISOU 898  $\mathsf{C}$ TYR 122 1833 1412 1439 89 -218 8 8 899 ATOM 0 TYR 122.4.395 30.507 48.117 1.000 14.25 ANISOU 899 0 TYR 122 1896 1861 1656 339 -242 2 1 6 ATOM 900 N PHE 123 2.224 30.269 47.573 1.000 11.28 123 1950 ANISOU 900 N PHE 1297 1041 6 -151 185 901 123 2.482 MOTA CAPHE 29.151 46.665 1.000 12.08 ANISOU 901 PHE CA 123 1731 1219 1640 64 - 60 2 6 ATOM 902 CB PHE 46.024 123 1.139 28.719 1.000 13.86 123 2048 ANISOU 902 CB PHE 1550 1666 -104 -276 -82ATOM 903 CG 123 1.311 PHE 27.516 45.099 1.000 14.44 ANISOU 903 123 2173 CG PHE 1677 1637 142 -475 - 94ATOM 904 CD1 PHE 123 1.281 26.234 1.000 13.64 45.614 ANISOU 904 CD1 PHE 123 1857 1563 1764 -42 -702 - 236905 CD2 PHE ATOM 123 1.511 27.664 43.729 1.000 13.81 ANISOU 905 CD2 PHE 123 1450 2164 1634 -420 -295 -248 ATOM 906 CE1 PHE 123 1.468 25.141 44.795 1.000 17.16 CE1 PHE ANISOU 906 123 2282 1819 130 -855 - 644 2418 CE2 PHE ATOM 907 123 1.715 26.559 42.916 1.000 18.31 ANISOU 907 CE2 PHE 123 2098 2657 2201 -1053 172 -845 ATOM 908 123 1.706 PHE CZ25.295 43.445 1.000 16.71 ANISOU 908 PHE CZ123 1442 2382 2526 -306 - 1077-36 909 ATOM 123 3.489 C PHE 29.511 45.581 1.000 13.48 ANISOU 909 C PHE 123 2004 1472 1645 236 157 1 8 910 ATOM 0 PHE 123 4.424 28.768 45.242 1.000 13.07 ANISOU 910 0 PHE 123 1591 1498 42 - 78 - 1721876 911 ATOM ASP N 124 3.294 30.684 44.948 1.000 13.83 ANISOU 911 ASP N 124 1490 1575 2189 51 207 288 ATOM 912 ASP CA 124 4.207 31.036 43.861 1.000 13.75 ANISOU 912 124 1505 CAASP 1330 2389 398 344 458 913 ATOM CB ASP 124 3.708 32.352 43.242 1.000 18.95 ANISOU 913 124 2650 CB ASP 1970 2580 656 -63 926 ATOM 914 124 4.470 CG ASP 32.708 41.989 1.000 27.54 ANISOU 914 CG ASP 124 5327 2099 3036 -123 939 880 OD1 ASP 915 ATOM 124 4.541 31.904 41.023 1.000 37.04

3225

4485

108

2616 - 331

124 6362

OD1 ASP

ANISOU 915

- 120 -ATOM 916 33.843 42.011 1.000 32.60 OD2 ASP 124 4.985 OD2 ASP ANISOU 916 124 4724 3509 4151 -1539 234 8 5 1 917 ATOM 124 5.645 31.164 44.328 1.000 14.49 C ASP ANISOU 917 C ASP 124 1493 1721 2293 327 485 482 918 ATOM ASP 30.721 43.674 1.000 14.52 124 6.591 ANISOU 918 124 1477 0 ASP 1363 2679 289 497 307 919 31.777 45.499 1.000 14.03 NARG ATOM 125 5.866 ARG 125 1501 ANISOU 919 N 2558 1271 353 398 414 920 125 7.214 CAATOM 46.044 1.000 16.40 ARG 31.863 ANISOU 920 ARG CA125 1642 1625 2963 178 226 194 921 C. **ARG** 30.494 46.346 1.000 14.69 ATOM: 125 7.828 ANISOU 921 125 1396 C ARG 1688 2496 232 -25 153 125 8.999 922 30.245 46.034 1.000 14.10 ATOM 0 ARG ANISOU 922 125 1279 0 ARG 1656 2424 7 - 205 - 201ATOM 923 ARG 125 7.213 32.705 47.318 1.000 18.13 CBANISOU 923 125 1950 CBARG 1902 3035 787 -81 4 6 125 7.045 CG ARG ATOM 924 34.193 47.041 1.000 23.51 ANISOU 924 CG ARG 125 2232 4919 1780 883 -36 - 225925 CDATOM 34.815 46.694 1.000 29.33 ARG 125 8.391 ANISOU 925 CDARG 125 3596 2824 -667 237 -1874724 MOTA 926 125.8.194 36.262 NEARG 46.803 1.000 32.99 ANISOU 926 ARG NE 125 4350 2766 5418 -678 -1642 156 927 MOTA CZARG 37.153 47.495 1.000 27.38 125 8.868 ANISOU 927 5353 CZARG 125 2292 2758 -276 -580 -246NH1 ARG ATOM 928 125 9.916 36.821 48.235 1.000 38.55 ANISOU 928 NH1 ARG 125 4611 3604 6433 449 -2476 -669 929 125 8.491 NH2 ARG MOTA 38.423 47.442 1.000 30.26 ANISOU 929 NH2 ARG 4865 125 4062 2570 -369 -835 3 6 3 ATOM 930 126 7.065 29.573 46.920 1.000 12.36 N GLN ANISOU 930 1376  $\mathbf{N}$ GLN 126 1316 2002 248 -63 - 264ATOM 931 GLN 28.201 47.153 1.000 13.39 CA126 7.524 1999 ANISOU 931 126 1765 CA GLN 1323 219 -355 - 377 AGLN 126 6.363 932 ATOM 27.455 47.828 0.500 16.24 СB AGLN 126 2422 ANISOU 932 2357 CB1391 188 202 - 192 AGLN 126 6.149 ATOM 933 CG 27.758 49.284 0.500 18.83 ANISOU 933 AGLN 126 2761 CG 2021 2371 68 233 - 210 27.146 50.298 0.500 23.94 934 ATOM CDAGLN 126 7.077 ANISOU 934 CDAGLN 126 3578 2745 2774 -604 -757 3 3 OE1 AGLN 126 7.181 27.683 51.419 0.500 35.94 ATOM 935 OE1 AGLN 126 6788 ANISOU 935 3731 3136 -578 -1567 -478 936 NE2 AGLN 126 7.774 26.055 50.008 0.500 24.63 ATOM ANISOU 936 NE2 AGLN 126 4491 1118 3751 -881 -2407 462 MOTA 937 BGLN 126 6.525 27.417 48.018 0.500 13.36 CB ANISOU 937 BGLN 126 1695 CB 1137 2245 602 -114 - 255ATOM 938 27.750 49.497 0.500 18.28 CG BGLN 126 6.604 ANISOU 938 BGLN 126 2537 CG 2257 2153 -68 -176 - 105939 ATOM CDBGLN 126 5.442 27.237 50.319 0.500 18.42 ANISOU 939 CD BGLN 126 2227 2573 2198 344 -159 1 0 6 OE1 BGLN 126 5.605 ATOM 940 26.442 51.242 0.500 25.36 ANISOU 940 OE1 BGLN 126 3289 3517 2828 -100 -223 9 5 3 941 NE2 BGLN 126 4.231 ATOM 27.685 50.003 0.500 25.02 NE2 BGLN 126 2427 ANISOU 941 2669 4413 1004 -83 -298 ATOM 942 126 7.860 27.448 45.861 1.000 12.95 GLN ANISOU 942 GLN 126 1506 1434 1979 307 -372 - 366 MOTA 943 26.721 45.748 1.000 11.66 0 GLN 126 8.859 ANISOU 943 0 GLN 126 1461 1142 1827 -85 159 182 944 ATOM TYR 127 6.960 27.578 44.868 1.000 11.61 N ANISOU 944 127 1400 1276 TYR N 1735 146 -168 - 10 ATOM 945  $\mathsf{C}\mathsf{A}$ TYR 127 7.152 26.869 43.585 1.000 11.21 ANISOU 945 CATYR 127 1469 1242 1550 -92 -40 192 MOTA CB 127 5.901 946 TYR 26.940 42.724 1.000 11.82

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- 121 -ANISOU 946 127 1346 CB TYR 1655 1491 -13 82 4 7 947 ATOM CG 127 5.791 TYR 26.069 1.000 11.49 41.496 ANISOU 947 127 1278 CG TYR 1428 1660 -4 - 4 1 0948 127 6.550 ATOM CD1 TYR 24.928 41.270 1.000 11.28 ANISOU 948 CD1 TYR 127 1030 1334 1921 -87 -100 3 3 ATOM CE1 TYR 127 6.406 949 40.115 1.000 11.47 24.153 ANISOU 949 CE1 TYR 127 1164 1167 2027 -53 2 1 -51 CD2 TYR 127 4.871 ATOM 950 26.410 40.500 1.000 11.98 ANISOU 950 CD2 TYR 127 1677 1093 1784 204 -219 - 100CE2 TYR MOTA 951 127 4.715 25.655 39.357 1.000 11.37 CE2 TYR ANISOU 951 127 1539 1118 1665 -68 - 73 140 952 ATOM CZTYR 127 5.494 24.508 39.163 1.000 11.02 ANISOU 952 CZ127 1202 TYR 1226 1760 91 48 - 125 953 ATOM OH 127 5.379 TYR 23.720 38.030 1.000 11.57 ANISOU 953 127 1547 OH TYR 1138 1712 94 177 - 34 954 ATOM C TYR 127 8.386 27.392 42.882 1.000 10.83 ANISOU 954 C TYR 127 1296 989 1830 230 -43 3 7 8 ATOM 955 0 TYR 127 9.185 26.605 42.375 1.000 10.86 ANISOU 955 127 1292 0 TYR 1232 1603 164 -237 - 42ATOM 956 THR 128 8.565 N 28.716 42.865 1.000 10.98 ANISOU 956 128 1554  $\mathbf{N}$ THR 976 1642 212 -9 5 5 7 ATOM 957 CA128 9.766 THR 29.305 42.295 1.000 11.80 ANISOU 957 CA128 1686 THR 1125 1673 -47-169 3 8 6 958 ATOM CB THR 128 9.605 42.378 1.000 12.66 30.849 ANISOU 958 128 1873 CB THR 1074 1864 -52 -233 5 2 1 128 8.530 ATOM 959 OG1 THR 41.517 1.000 16.74 31.286 ANISOU 959 OG1 THR 128 2223 1597 124 -457 9 9 8 2542 ATOM 960 CG2 THR 128 10.878 31.510 41.893 1.000 16.54 CG2 THR ANISOU 960 128<sup>2</sup>1871 778 3635 262 655 1 3 8 ATOM 961 C THR 128 11.040 28.828 42.964 1.000 11.26 ANISOU 961 C THR 128 1562 980 1738 -71 -162 148 ATOM 962 0 THR 128 11.995 28.458 42.258 1.000 12.16 ANISOU 962 128 1769 0 THR 1758 1092 17 26 279 ATOM 963 N ALA 129 11.083 44.300 1.000 10.39 28.802 ANISOU 963 129 1183 ALA N 1001 1763 70 -118 147 · ATOM 964 129 12.273 ÇA ALA 28.386 45.037 1.000 10.59 129 1206 ANISOU 964 CAALA 945 1873 -69 -170 281 ATOM 965 CB 129 12.113 ALA 28.603 46.536 1.000 12.46 ANISOU 965 129 2113 CBALA 851 1769 82 -218 ATOM 966 C ALA 129 12.575 26.906 44.802 1.000 11.35 ANISOU 966 C ALA 129 1258 883 2170 -16 -141 ATOM 967 26.485 44.641 1.000 10.93 ALA 129 13.738 ANISOU 967 129 1202 0 ALA 1157 1796 -36 -213 1 2 1 ATOM 968 SER N 130 11.519 26.086 44.750 1.000 12.27 ANISOU 968 N SER 130 1280 984 2398 -65 -1 - 24ATOM 969 SER 130 11.682 CA24.650 44.512 1.000 10.89 ANISOU 969 CASER 130 1623 876 1638 -85 44 3 7 0 ATOM ASER 130 10.342 970 CB23.940 44.716 0.500 10.08 ANISOU 970 ASER 130 1432 CB603 1793 213 247 413 ATOM ASER 130 9.771 971 OG 24.063 46.006 0.500 9.12 ANISOU 971 ASER 130 1021 OG 651 1792 911 - 143ATOM 972 BSER 130 10.364 CB 23.919 44.765 0.500 10.60 ANISOU 972 BSER 130 1687 CB 822 1521 -45 318 158 ATOM BSER 130 9.418 973 OG 24.098 43.734 0.500 16.22 ANISOU 973 BSER 130 1717 0G 1289 3156 137 -525 3 4 8 ATOM 974 C SER 130 12.214 24.373 43.110 1.000 10.53 ANISOU 974 C 130 1586 SER 733 1684 -166 210 484 ATOM 975 0 130 13.137 SER 23.532 42.942 1.000 11.17 ANISOU 975 0 130 1385 SER 1012 1849 -151 -95 140 ATOM 976 N 131 11.680 ARG 25.044 42.079 1.000 10.46 ANISOU 976 131 1578 861 1534 ARG -87 -66 9 9

- 122 -977 24.839 MOTA CAARG 131 12.260 40.742 1.000 10.60 ANISOU 977 ARG 1110 CA131 1480 1438 61 - 288978 ARG 131 11.426 25.553 39.679 ATOM CB 1.000 12.99 ANISOU 978 ARG 131 1893 1369 CB 1673 63 - 525276 ATOM 979 CG ARG 131 10.003 25.065 39.431 1.000 13.64 ANISOU 979 131 1707 1735 CG ARG 1742 335 -559 - 8625.669 ARG 131 9.349 38.206 1.000 17.71 ATOM 980 CDANISOU 980 131 2078 1973 2677 CDARG 81 - 983 701 ATOM 981 ARG 38.015 NE 131 9.453 27.113 1.000 19.76 ANISOU 981 NE 131 2716 2034 ARG 2757 -25 -52571338.568 1.000 21.24 ARG 131 8.629 28.004 ATOM 982 CZANISOU 982 CZ131 3688 1878 ARG 2503 -8 - 1286 4 7 NH1 ARG 27.634 39.366 1.000 21.32 983 131 7.631 ATOM ANISOU 983 NH1 ARG 131 2792 3142 -486 -667 5 7 2166 ATOM 984 NH2 ARG 29.310 38.361 1.000 27.83 131 8.771 NH2 ARG ANISOU 984 131 4649 1822 -422 5 6 1 4103 -90 ATOM 985 25.323 40.688 1.000 10.42 C ARG 131 13.714 ANISOU 985  $\mathsf{C}$ ARG 131 1542 1078 1339 50 -103 1 ATOM 986 24.683 40.080 1.000 10.94 0 131 14.568 ARG ANISOU 986 0 ARG 131 1544 1105 1506 177 -134 4 2 132 14.028 ATOM 987 N ALA 26.438 41.343 1.000 10.97 ANISOU 987 N ALA 132 1477 1129 1563 74 - 364 - 45 ATOM 988 ALA 132 15.379 26.983 41.343 CA1.000 11.10 CA 132 1539 ANISOU 988 ALA 944 1735 9 -102 9 7 1.000 12.82 ALA ATOM 989 CB 28.344 42.048 132 15.429 ANISOU 989 ALA CB 1987 -48 132 1711 1171 -248 - 198ATOM 990 ALA 132 16.393 26.045 C 41.995 1.000 11.55 ALA 132 1085 -197 305 745 ANISOU 990 1107 2197 C MOTA ALA 25.832 991 0 132 17.481 41.432 1.000 11.81 ANISOU 991 0 1599 ALA 1809 132 1081 -204 17 - 9ATOM 992 43.175 N 133 16.061 VAL 1.000 11.16 : 25.490 ANISOU 992 N VAL 133 1260 1356 1623 -148 51 3 5 0 133 17.011 24.587 ATOM 993 CA VAL 43.840 1.000 11.62 ANISOU 993 CA 133 1505 1380 -69 -29789VAL 1529 ATOM 994 CB VAL 133 16.738 1.000 12.14 24.418 45.344 ANISOU 994 CB VAL 133 1376 -25 364 1564 1674. -74 ATOM 995 CG1 VAL 133 15.550 23.501 45.608 1.000 14.96 133 1705 ANISOU 995 CG1 VAL 2316 1662 **-**706 8 CG2 VAL MOTA 996 133 17.981 23.864 46.033 1.000 15.63 ANISOU 996 CG2 VAL 133 1755 1845 -677 5 5 1 2340 -341 997 C VAL 133 17.079 23.268 43.065 1.000 11.71 ATOM ANISOU 997 C 133 1376 VAL 1363 1711 -24 ATOM 998 O VAL 133 18.198 22.733 42.925 1.000 11.55 ANISOU 998 1545 VAL 133 1391 1453 -4 -116 398 ALA 134 15.982 22.758 42.480 1.000 12.87 999 N MOTA ALA 134 1399 ANISOU 999 N 1517 1973 28 - 334 - 228ALA 134 16.084 21.557 41.621 1.000 10.57 ATOM 1000 CA ALA 134 1106 ANISOU 1000 CA 1220 1691 153 -298 9 6 1001 CB ALA 134 14.699 21.096 41.186 1.000 12.20 MOTA ANISOU 1001 CB ALA 134 1254 1589 1794 35 - 303 - 127ATOM ALA 134 16.968 21.797 40.399 1.000 12.58 1002 C ANISOU 1002 C ALA 134 1393 1399 1987 272 -4 277ATOM 1003 0 ALA 134 17.712 20.924 39.970 1.000 11.01 ANISOU 1003 O ALA 134 1254 83 - 268 2 6. 1358 1574 ARG 135 16.908 22.995 39.809 1.000 12.03 ATOM 1004 N ANISOU 1004 N ARG 135 1517 -327 8 7 1230 1824 -62 1005 CA ARG 135 17.773 23.353 38.676 1.000 13.23 ATOM ANISOU 1005 CA ARG 135 1854 1158 -270 -209 1 6 1 2015 1006 CB ARG 135 17.393 24.734 38.170 1.000 14.57 MOTA ANISOU 1006 CB ARG 135 2203 1339 1994 -45 -541 2 2 2 ATOM 1007 CG ARG 135 17.753 25.160 36.797 1.000 19.22

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- 123 -ANISOU 1007 CG 135 4204 ARG 1120 -490 -433 1 5 0 1980 1008 CD ATOM ARG 135 17.237 26.563 36.471 1.000 22.14 ANISOU 1008 CD ARG 135 4046 1500 2868 -159 315 1009 NE ATOM ARG 135 15.831 26.607 36.077 1.000 22.66 135 4239 ANISOU 1009 NE ARG 1404 2965 -94 47 2 5 7 1010 CZ ATOM ARG 135 14.802 27.184 36.684 1.000 21.69 ANISOU 1010 CZ 135 4004 ARG 1906 2333 92 - 506 6 4 1011 NH1 ARG ATOM 135 14.917 27.843 37.833 1.000 22.26 ANISOU 1011 NH1 ARG 135 4114 2532 460 -833 3 4 1 1812 1012 NH2 ARG ATOM 135 13.582 27.113 1.000 22.31 36.149 ANISOU 1012 NH2 ARG 135 4000 2243 2234 -544 -419 8 1013 C ATOM ARG 135 19.251 23.275 39.057 1.000 12.70 ANISOU 1013 C ARG 135 1742 1264 1821 -119 -16 430 ATOM 1014 0 ARG 135 20.069 22.818 38.238 1.000 14.67 ANISOU 1014 O 135 2133 ARG 1529 1910 19 169 3 9 1 ATOM 1015 N 136 19.572 GLU 23.712 40.266 1.000 12.15 136 1423 ANISOU 1015 N GLU 1372 1820 -3670 4 3 0 136 20.960 ATOM 1016 CA GLU 23.630 1.000 14.52 40.763 ANISOU 1016 CA GLU 136 1622 1701 2194 -90 -197 3 7 1 ATOM 1017 CB 136 21.212 GLU 41.981 24.513 1.000 15.59 ANISOU 1017 CB GLU 136 1502 1781 2642 14 -231 ATOM 1018 CG GLU 136 21.064 26.020 41.783 1.000 18.01 ANISOU 1018 CG 136 2010 GLU 1762 3071 -232 -153 1 2 6 ATOM 1019 CD GLU 136 21.798 26.484 40.537 1.000 20.18 ANISOU 1019 CD GLU 136 2071 2079 3519 -308 89 3 6 9 1020 OE1 GLU ATOM 136 22.987 26.148 40.394 1.000 24.64 ANISOU 1020 OE1 GLU 136 2060 2937 -262 4364 338 615 1021 OE2 GLU ATOM 136 21.195 27.150 39.670 1.000 24.19 ANISOU 1021 OE2 GLU 136<sup>-2</sup>479 2327 4385 -381 317 1426 1022 C ATOM 136 21.364 GLU 22.186 41.076 1.000 14.00 ANISOU 1022 C GLU 136 1338 2361 1619 -112 -442 2 2 3 ATOM 1023 0 GLU 136 22.508 21.781 40.833 1.000 13.86 ANISOU 1023 O GLU 136 1366 1890 2009 -100 -287 3 2 9 1024 N MOTA VAL 137 20.472 21.338 41.580 1.000 11.78 ANISOU 1024 N VAL 137 1309 1451 1715 148 -223 8 5 MOTA 1025 CA 137 20.753 VAL 19.896 41.771 1.000 12.49 ANISOU 1025 CA VAL 137 1369 152.2 1853 240 -69 2 8 9 ATOM 1026 CB VAL 137 19:560 19.165 1.000 12.41 42.429 ANISOU 1026 CB VAL 137 1422 1424 1869 -67 -85 - 2041027 CG1 VAL ATOM 137 19.728 17.634 42.401 1.000 12.55 ANISOU 1027 CG1 VAL 137 1371 1508 1892 182 185 111 ATOM 1028 CG2 VAL 19.607 43.852 1.000 11.35 137 19.355 ANISOU 1028 CG2 VAL 137 1461 1281 1572 182 -254 2 8 8 ATOM 1029 C VAL 137 21.100 19.241 40.435 1.000 12.48 ANISOU 1029 C VAL 137 1202 1428 2113 150 -16 8 5 1030 O ATOM VAL 137 22.057 18.462 40.287 1.000 13.03 ANISOU 1030 O VAL 137 1021 1683 2249 149 1 1 4 6 ATOM 1031 N LEU 138 20.309 19.562 39.401 1.000 10.28 ANISOU 1031 N LEU 138 1198 881 1829 -15 158 2 2 6 1032 CA LEU ATOM 19.029 38.066 1.000 12.48 138 20.571 ANISOU 1032 CA LEU 138 1312 1408 2024 110 273 - 52 ATOM 1033 CB 138 19.398 LEU 19.358 37.130 1.000 11.81 ANISOU 1033 CB 138 1260 LEU 1586 1642 -20 383 4 3 ATOM 1034 CG LEU 138 18.036 18.726 37.457 1.000 10.77 ANISOU 1034 CG LEU 138 1391 1397 1304 -83 219 213 1035 CD1 LEU MOTA 138 16.916 19.324 36.596 1.000 12.72 ANISOU 1035 CD1 LEU 138 1416 1587 1829 -59 -25 173 1036 CD2 LEU MOTA 138 18.052 17.207 1.000 14.32 37.320 ANISOU 1036 CD2 LEU 138 1986 1390 2065 -79 296 370 MOTA 1037 C LEU 138 21.903 19.525 37.505 1.000 13.61 ANISOU 1037 C 138 1305 LEU -65 2026 1840 174 5

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1038 0
                                  18.760
ATOM
                LEU
                     138 22.695
                                         36.920 1.000 14.97
ANISOU 1038 O
                LEU
                     138 1125
                                  2247
                                                 105
                                          2313
                                                       234 178
ATOM
       1039 N
                     139 22.184
                ARG
                                  20.816
                                         37.614 1.000 13.26
ANISOU 1039 N
                ARG
                                  2046
                     139 1432
                                         1561
                                                 -155 219 317
ATOM
       1040 CA
                ARG
                     139 23.397
                                  21.372
                                         37.085
                                                 1.000 14.71
                     139 1648
ANISOU 1040 CA
                ARG
                                          2000
                                  1941
                                                  -27
                                                       502 447
                     139 24.636
ATOM
       1041 C
                ARG
                                  20.815
                                         37.775
                                                 1.000 15.16
ANISOU 1041 C
                                                 -158 324 116
                ARG
                     139 1425
                                  2101
                                          22.35
       1042 0
                ARG
                     139 25.650
                                         37.166 1.000 18.15
ATOM
                                  20.495
ANISOU 1042 O
                ARG
                     139 1628
                                  2581
                                          2688
                                                  18 612 3 3 9
                                 22.926
       1043 CB
                ARG
                     139 23.394
                                         37.206 1.000 19.67
ATOM
ANISOU 1043 CB
                ARG
                     139 1749
                                  1923
                                          3803
                                                 -196 186 252
ATOM
       1044 CG
                ARG
                     139 24.418
                                  23.487
                                         36.237
                                                 1.000 28.66
ANISOU 1044 CG
                ARG
                     139 3924
                                  2584
                                          4383
                                                 -2305 882 - 563
ATOM
       1045 CD
                ARG
                     139 24.245
                                         36.111 1.000 39.58
                                  24.997
ANISOU 1045 CD
                ARG
                                  2389
                     139 6801
                                          5849
                                                  -3273 119 - 306
       1046 NE
                                         37.210 1.000 47.91
ATOM
                ARG
                     139 24.910
                                  25.660
ANISOU 1046 NE
                ARG
                     139 9548
                                  2435
                                          6222
                                                  -2157 -1331 -708
ATOM
       1047 CZ
                     139 24.493
                ARG
                                  26.682
                                         37.928 1.000 45.42
                ARG
ANISOU 1047 CZ
                     139 6941
                                  4516
                                          5802
                                                  -882 -2118 -1238
       1048 NH1 ARG
                     139 23.316
ATOM
                                  27.273
                                         37.722 1.000 64.33
ANISOU 1048 NH1 ARG
                     139 7248
                                  8153
                                          9039
                                                 93 - 2965 - 980
       1049 NH2 ARG
ATOM
                     139 25.309
                                  27.109 38.888 1.000 32.62
ANISOU 1049 NH2 ARG
                     139 5020
                                  4758
                                          2616
                                                  -2746 590 1 6 7
       1050 N
                ALA
ATOM
                     140 24.562
                                  20.684 39.096 1.000 14.85
ANISOU 1050 N
                ALA
                     140 1287
                                  2204
                                          2151
                                                  -517 - 26 - 46
       1051 CA
                ALA
ATOM
                     140 25.730
                                  20.257 39.856 1.000 15.80
ANISOU 1051 CA
                ALA
                     140 989 2649
                                      2366
                                              -309 -9 -401
       1052 CB
ATOM
                     140 25.444
                                  20.442 41.330 1.000 19.36
                ALA
ANISOU 1052 CB
                ALA
                     140 2685
                                  2447
                                          2222
                                                  243
                                                       -435 - 480
       1053 C
ATOM
                     140 26.111
                                  18.806
                                         39.584 1.000 16.86
                ALA
                                          2054
ANISOU 1053 C
                ALA
                     140 1555
                                  2795
                                                  12 -186 - 458
ATOM
       1054 O
                ALA
                                  18.403
                                         39.796
                     140 27.258
                                                 1.000 18.90
ANISOU 1054 O
                ALA
                     140 1538
                                  2686
                                          2958
                                                  -21
                                                        60 1 4 5
                                  18.025
MOTA
       1055 N
                THR
                                                 1.000 17.53
                     141 25.147
                                         39.098
ANISOU 1055 N
                THR
                     141 1779
                                  2532.
                                          2350
                                                  -528 218 -108
       1056 CA
                                  16.625
ATOM
                THR
                     141 25.340
                                          38.765
                                                 1.000 15.59
ANISOU 1056 CA
                THR
                                  2401
                                          2268
                                                  -192 -95 291
                     141 1256
       1057 CB
ATOM
                THR
                     141 24.207
                                  15.735
                                         39.343
                                                  1.000 14.77
ANISOU 1057 CB
                THR
                     141 1238
                                  2200
                                          2172
                                                  155
                                                        282 3 0 1
       1058 OG1 THR
ATOM
                    141 22.946
                                 16.168 38.849 1.000 12.47
ANISOU 1058 OG1 THR
                                          1926
                     141 1249
                                  1565
                                                       295 476
                                                  -31
       1059 CG2 THR
MOTA
                     141 24.167
                                  15.818 40.859 1.000 14.82
ANISOU 1059 CG2 THR
                     141 1394
                                  2077
                                                  135
                                          2160
                                                        -47 177
       1060 C
ATOM
                THR
                                  16.374 37.257 1.000 16.11
                     141 25.423
ANISOU 1060 C
                THR
                     141 1732
                                  2046
                                                  303
                                          2343
                                                        583 325
       1061 0
ATOM
                THR
                                  15.235
                     141 25.432
                                         36.778 1.000 17.55
ANISOU 1061 O
                THR
                     141 1991
                                  2104
                                          2573
                                                  237
                                                        555 249
       1062 N
ATOM
                     142 25.474
                                  17.416
                                         36.446 1.000 17.74
                GLY
ANISOU 1062 N
                GLY
                      142 2127
                                  2197
                                          2416
                                                  303
                                                        260 501
       1063 CA
ATOM
                GLY
                      142 25.611
                                          34.987
                                  17.263
                                                  1.000 17.32
                GLY
ANISOU 1063 CA
                      142 1642
                                  2494
                                          2447
                                                  -160 453 517
ATOM
       1064 C
                GLY
                      142 24.426
                                  16.556 34.358 1.000 16.37
ANISOU 1064 C
                GLY
                      142 1619
                                                        472 4 2
                                  1893
                                          2710
                                                  261
ATOM
       1065 O
                GLY
                      142 24.654
                                  15.824 33.379 1.000 18.43
ANISOU 1065 O
                GLY
                      142 2243
                                  2558
                                          2201
                                                  57 798 1 6 3
ATOM
       1066 N
                 THR
                      143 23.232
                                  16.738
                                         34.907 1.000 13.99
ANISOU 1066 N
                 THR
                      143 1531
                                  1429
                                          2356
                                                  83 430 3 5 0
       1067 CA
ATOM
                 THR
                      143 22.049
                                  16.003 34.472 1.000 14.69
ANISOU 1067 CA
                 THR
                      143 1768
                                  1591
                                          2223
                                                  8 342 9 3
MOTA
       1068 CB
                 THR
                                  15.584 35.700 1.000 15.52
                      143 21.208
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- 125 -ANISOU 1068 CB THR 143 1457 1653 2785 55 419 5 2 9 1069 OG1 THR ATOM 143 22.037 14.784 36.573 1.000 14.63 ANISOU 1069 OG1 THR 143 1296 1792 2471 52 434 3 6 9 1070 CG2 THR ATOM 143 20.044 35.231 1.000 14.24 14.738 ANISOU 1070 CG2 THR 143 1761 1669 1981 3 379 1 9 2 ATOM 1071 C THR 143 21.135 16.785 33.532 1.000 13.96 ANISOU 1071 C THR 143 1553 1708 2044 128 479 - 131 1072 0 ATOM THR 143 20.642 17.828 33.923 1.000 15.65 ANISOU 1072 O THR 143 2374 1580 1995 315 486 5 5 ATOM 1073 N GLU 144 20.928 16.279 1.000 15.32 32.322 GLU ANISOU 1073 N 144 1734 1904 2184 -156 260 -271 ATOM 1074 CA GLU 144 19.917 31.362 1.000 17.30 16.693 ANISOU 1074 CA GLU 144 1686 2470 2417 -377 152 106 1075 C MOTA GLU 15.693 144 18.774 31.292 1.000 16.84 ANISOU 1075 C GLU 144 1633 2380 2386 -298 313 -242 1076 0 GLU ATOM 144 18.922 30.680 1.000 16.71 14.631 ANISOU 1076 O GLU 144 1470 2057 2821 -43 610 1077 CB ATOM GLU 16.856 144 20.539 29.970 1.000 21.91 ANISOU 1077 CB GLU 144 2747 3417 2162 -150831 - 8MOTA 1078 CG GLU 144 19.568 28.825 1.000 37.93 17.063 ANISOU 1078 CG GLU 144 6652 4374 3385 -2057 -2082 1767 1079 CD MOTA GLU 18.507 28.466 1.000 43.55 144 19.293 ANISOU 1079 CD GLU 4258 144 7869 4419 -2497 -2259 2129 1080 OE1 GLU ATOM 144 19.602 19.365 29.326 1.000 51.81 ANISOU 1080 OE1 GLU 144 9843 4613 5230 -3180 -832 1126 1081 OE2 GLU ATOM 144 18.766 18.798 27.367 1.000 40.12 ANISOU 1081 OE2 GLU 144 5551 6029 3662 -285 -115 2660 ATOM 1082 N PRO 145 17.620 15.959 31.908 1.000 14.29 ANISOU 1082 N PRO 145 1634 1364 2432 -4 208 265 ATOM 1083 CD 145 17.256 PRO 32.718 1.000 14.14 17.136 ANISOU 1083 CD 145 1735 PRO 1778 1859 -55 32 1 6 7 ATOM 1084 CA 145 16.507 PRO 15.000 31.807 1.000 13.72 ANISOU 1084 CA PRO 145 1484 1391 2337 66 173 4 6 6 1085 CB ATOM PRO 145 15.406 15.701 32.606 1.000 14.20 ANISOU 1085 CB PRO 145 1459 1636 2302 161 -41 ATOM 1086 CG PRO 145 16.132 16.608 33.561 1.000 14.43 ANISOU 1086 CG 145 1796 PRO 2007 1679 -23 -42 4 4 9 ATOM 1087 C PRO 145 16.076 14.794 30.372 1.000 15.18 ANISOU 1087 C 145 1745 PRO 1665 2359 -192 231 ATOM -1088 O PRO 145 16.178 15.685 29.509 1.000 15.40 ANISOU 1088 O 145 2430 PRO 1511 1910 -85 613 ATOM 1089 N ASP 13.613 30.070 1.000 15.79 146 15.544 ANISOU 1089 N ASP 146 2019 1611 2367 -191 666 8 1 1090 CA MOTA ASP 13.366 28.773 1.000 16.74 146 14.918 ANISOU 1090 CA ASP 146 2095 1759 2506 -348 575 - 77 MOTA 1091 CB ASP 11.966 28.727 1.000 18.99 146 14.300 ANISOU 1091 CB ASP 146 2508 1729 2977 -323 780 -439 1092 CG ATOM ASP 146 13.504 11.784 27.444 1.000 27.04 ANISOU 1092 CG ASP 146 4012 2450 3813 -720 -229 -805 1093 OD1 ASP ATOM 146 12.295 12.121 27.409 1.000 38.65 ANISOU 1093 OD1 ASP 146 3943 4889 5852 -59.5 -1282 -3231094 OD2 ASP ATOM 11.311 26.466 1.000 39.95 146 14.091 ANISOU 1094 OD2 ASP 146 6913 5052 3214 16 0 -1182 1095 C ATOM ASP 146 13.860 14.441 28.552 1.000 16.65 ANISOU 1095 C ASP 146 2461 1904 1961 -128 580 -40ATOM 146 13.041 1096 0 ASP 14.605 29.457 1.000 15.67 ANISOU 1096 O ASP 146 2110 1935 -334 381 -4201908 ATOM 1097 N GLY 147 13.871 15.149 27.429 1.000 20.60 ANISOU 1097 N GLY 147 3484 2416 1927 -26 419 129 ATOM 1098 CA GLY 147 12.903 16.212 27.155 1.000 18.06 ANISOU 1098 CA 147 2771 GLY 2451 1638 -382 98 9 3

- 126 -MOTA 1099 C GLY 17.574 27.609 1.000 18.73 147 13.361 GLY ANISOU 1099 C 2195 147 2836 2085 -524 143 ATOM 1100 O GLY 147 12.676 18.570 27.282 1.000 18.34 ANISOU 1100 O GLY 1687 -413389 147 2865 2416 -72 148 14.498 ATOM 1101 N GLY 17.634 28.316 1.000 16.35 1506 ANISOU 1101 N GLY 148 2936 1772 -157 142 8 8 18.889 1102 CA ATOM GLY 148 15.116 28.747 1.000 15.34 55 450 - 26 ANISOU 1102 CA GLY 148 2723 1829 1279 ATOM 1103 C GLY 148 14.768 19.339 30.144 1.000 12.97 ANISOU 1103 C GLY 148 2231 1416 1280 -93  $-62 \quad 4 \quad 0 \quad 7$ GLY ATOM 1104 0 148 13.769 18.930 1.000 13.79 30.771 ANISOU 1104 O GLY 1561 148 2301 1376 -164 88 3 2 3 1105 N ATOM VAL 149 15.604 20.224 30.718 1.000 12.81 ANISOU 1105 N VAL 149 1815 1366 1686 155 -31 238 VAL 149 15.388 20.724 32.079 1.000 11.81 ATOM 1106 CA ANISOU 1106 CA VAL 149 1333 1765 54 -92 1 2 9 1390 1107 CB ATOM VAL 149 16.594 21.636 32.480 1.000 11.97 ANISOU 1107 CB VAL 149 1136 1696 1717 -100 246 124 1108 CG1 VAL ATOM 149 16.358 22.336 33.802 1.000 15.26 ANISOU 1108 CG1 VAL 1922 149 1941 1936 -195 55 - 2231109 CG2 VAL ATOM 149 17.868 20.794 32.538 1.000 17.21 ANISOU 1109 CG2 VAL 149 1231 45 102 - 103 2045 3265 MOTA 1110 C 149 14.101 21.482 VAL 32.280 1.000 11.32 ANISOU 1110 C 149 1186 VAL 1303 1813 -78 131 479 33.253 1111 0 ATOM 149 13.378 21.218 VAL 1.000 12.35 ANISOU 1111 O VAL 149 1664 1423 1608 -71 229 167 ATOM 1112 N GLU 22.463 150 13.752 31.460 1.000 11.96 ANISOU 1112 N GLU 150 1347 1453 1746 29 - 36 4 2 0 150 12.592 23.286 31.815 1.000 10.90 ATOM 1113 CA GLU 150 1623 ANISOU 1113 CA GLU 1359 1159 118 0 4 0 5 ATOM 1114 CB GLU 150 12.608 24.601 30.999 1.000 17.60 ANISOU 1114 CB GLU 150 2530 1470 2687 181 -161 9 0 7 25.488 31.314 1.000 17.86 ATOM 1115 CG GLU 150 13.811 ANISOU 1115 CG 150 2744 GLU 797 3246 246 434 202 1116 CD ATOM 150 13.956 25.929 32.738 1.000 19.47 GLU ANISOU 1116 CD GLU 150 3018 1353 3027 -84 662 -97 1117 OE1 GLU 150 12.951 26.005 33.475 1.000 18.21 ATOM ANISOU 1117 OE1 GLU 150 3035 1512 2373 -178 -3215361118 OE2 GLU 150 15.109 26.237 33.122 1.000 22.59 ATOM ANISOU 1118 OE2 GLU 150 2993 1664 3927 -38 -150284ATOM 1119 C GLU 150 11.277 22.533 31.705 1.000 12.22 ANISOU 1119 C GLU 235 150 1429 1540 1676 147 - 5MOTA 1120 0 150 10.341 22.757 32.530 1.000 13.44 GLU ANISOU 1120 O GLU 150 1739 1474 1894 315 470 288 1121 N 151 11.118 21.625 30.742 1.000 11.88 ALA ATOM ANISOU 1121 N ALA 151 1783 1255 1477 94 45 253 ATOM 1122 CA ALA 20.844 30.698 1.000 13.82 151 9.881 ANISOU 1122 CA ALA 151 1744 2054 -100 -413 3 9 6 1454 1123 CB ALA 20.094 29.390 1.000 14.89 ATOM 151 9.739 ANISOU 1123 CB ALA 151 1489 2318 1851 22 - 269 - 35 1124 C MOTA ALA 19.864 31.867 1.000 12.71 151 9.792 ANISOU 1124 C 151 1448 1463 ALA .1920 93 41 424 MOTA 1125 O ALA 19.580 32.280 1.000 14.69 151 8.655 ANISOU 1125 O ALA -242 204 -108 151 1535 2114 1932 152 10.925 19.401 32.410 1.000 11.73 ATOM 1126 N PHE ANISOU 1126 N PHE 9 271 152 1598 1259 120 1598 1127 CA PHE MOTA 152 10.890 18.554 33.602 1.000 10.61 ANISOU 1127 CA PHE 152 1444 1061 1526 -33 34 1 6 0 1128 CB PHE ATOM 152 12.293 17.981 33.820 1.000 10.23 ANISOU 1128 CB PHE 152 1317 -144 207 410 1132 1437 1129 CG PHE 152 12.517 17.187 35.095 1.000 10.36 ATOM

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- 127 -ANISOU 1129 CG PHE 152 1388 1149 1399 147 276 -34 1130 CD1 PHE ATOM 152 12.036 15.896 35.229 1.000 11.24 ANISOU 1130 CD1 PHE 152 1479 1047 1743 114 -103 5 6 6 ATOM 1131 CD2 PHE 152 13.229 17.701 36.154 1.000 11.21 ANISOU 1131 CD2 PHE 152 1489 1319 1449 85 174 1 5 1 1132 CE1 PHE ATOM 152 12.252 15.163 1.000 10.80 36.380 ANISOU 1132 CE1 PHE 152 1400 1234 249 1467 -111 3 7 3 1133 CE2 PHE ATOM 152 13.431 16.992 37.341 1.000 11.82 ANISOU 1133 CE2 PHE 152 1709 1622 1160 414 250 -276 1134 CZ ATOM 152 12.932 PHE 15.717 37.457 1.000 11.97 ANISOU 1134 CZ 152 1651 PHE 1604 1293 296 170 -255 1135 C ATOM 152 10.430 PHE 19.292 34.858 1.000 12.24 ANISOU 1135 C 152 1754 PHE 1730 1168 339 8 4 -101136 0 MOTA 152 9.728 PHE 18.729 35.726 1.000 11.49 ANISOU 1136 O 152 1672 PHE 1142 1550 200 109 277 1137 N ATOM LEU 153 10.809 20.575 34.997 1.000 11.86 ANISOU 1137 N LEU 153 2030 1236 1240 -6 73 1 5 6 1138 CA 153 10.532 ATOM LEU 21.386 1.000 11.99 36.155 ANISOU 1138 CA 153 1890 LEU 1437 1229 **-165** 307 8 5 ATOM 1139 CB 153 11.654 LEU 22.420 36.353 1.000 12.81 ANISOU 1139 CB LEU 153 1691 1381 1794 -72 97 - 40ATOM 1140 CG LEU 153 13.059 21.910 36.592 1.000 12.87 ANISOU 1140 CG LEU 153 1762 1645 1483 146 269 6 4 1141 CD1 LEU ATOM 153 14.027 23.081 36.611 1.000 15.99 ANISOU 1141 CD1 LEU 153 1609 2006 2462 -49 450 - 431ATOM 1142 CD2 LEU 153 13.185 21.158 37.914 1.000 19.37 ANISOU 1142 CD2 LEU 153 3091 2462 1806 809 275 540 1143 C ATOM 153 9.179 LEU 22.084 36.123 1.000 12.96 ANISOU 1143 C 153 1728 LEU 1253 -336 360 -43 1943 ATOM 1144 0 153 8.709 LEU 22.506 37.193 1.000 13.24 ANISOU 1144 O LEU 153 1617 1302 -443 481 -182 2109 1145 N ATOM ASP 154 8.568 22.203 34.955 1.000 13.29 ANISOU 1145 N ASP 154 1643 1457 1951 60 517 2 8 0 ATOM 1146 CA ASP 22.671 154 7.195 34.764 1.000 14.21 ANISOU 1146 CA 154 1862 ASP 1255 2280 313 631 683 ATOM 1147 CB ASP 23.269 154 6.995 33.373 1.000 18.38 ANISOU 1147 CB ASP 154 2091 2156 2738 728 328 1475 ATOM 1148 CG 154 5.534 ASP 23.367 1.000 22.95 32.929 ANISOU 1148 CG ASP 154 2323 3543 2855 676 430 1501 1149 OD1 ASP ATOM 154 4.685 23.607 33.820 1.000 20.85 ANISOU 1149 OD1 ASP 154 2164 2368 3389 895 478 ATOM 1150 OD2 ASP 23.254 31.702 1.000 24.33 154 5.168 ANISOU 1150 OD2 ASP 154 2989 3146 3110 228 48 1128 1151 C ATOM 154 6.294 ASP 21.455 34.985 1.000 11.22 ANISOU 1151 C ASP 154 1594 1403 1265 147 410 123 ATOM 1152 0 ASP 154 6.043 20.729 34.015 1.000 13.31 ANISOU 1152 O ASP 154 2143 1728 1186 427 219 170 ATOM 1153 N CYS 155 5.891 21.220 36.233 1.000 9 . 9 1 ANISOU 1153 N 155 1425 CYS 1098 1243 -76 186 2 7 ATOM 1154 CA CYS 155 5.446 19.881 36.627 1.000 9 . 4 1 ANISOU 1154 CA CYS 155 1294 1168 1115 -13 154 172 ATOM 1155 CB CYS 155 6.635 19.171 37.269 1.000 10.64 ANISOU 1155 CB CYS 155 1276 1015 1753 28 - 51 - 122 1156 SG MOTA 155 7.316 CYS 19.819 38.797 1.000 12.01 ANISOU 1156 SG CYS 155 1376 1554 1633 -195 -199 9 5 ATOM 1157 C CYS 155 4.138 19.885 37.423 1.000 9.66 ANISOU 1157 C 155 1301 CYS 1355 115 1013 146 216 ATOM 1158 O CYS 155 3.215 37.064 1.000 11.61 20.645 ANISOU 1158 O CYS 155 1349 1386 1676 130 116 294 1159 N ATOM 156 4.021 GLU 38.442 1.000 10.26 19.033 ANISOU 1159 N 156 1263 GLU 1495 1139 -29 168 299

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ATOM 1160 CA GLU	156 2.778	18.787 39.173	1.000 9.04
ANISOU 1160 CA GLU	156 998 1160		
ATOM 1161 CB GLU	156 2.300	17.391 38.772	1.000 11.63
ANISOU 1161 CB GLU	156 1187	1348 1885	-67 -135 -190
ATOM 1162 CG GLU	·		1.000 14.29
ANISOU 1162 CG GLU	156 1741	1640 2049	-628 -507 5 0
ATOM 1163 CD GLU			1.000 17.90
ANISOU 1163 CD GLU ATOM 1164 OE1 GLU		2692 2336	-365 -686 1 3 7
ATOM 1164 OE1 GLU ANISOU 1164 OE1 GLU	156 -0.220 156 1429	18.241 38.024 2973 2884	1.000 19.17 -632 -270 253
ATOM 1165 OE2 GLU		18.198 35.858	1.000 22.03
ANISOU 1165 OE2 GLU	156 2449		-243 -721 9 2 4
ATOM 1166 C GLU	156 2.961		1.000 9 . 21
ANISOU 1166 C GLU	156 1166	1135 1197	-26 239 183
ATOM 1167 0 GLU	156 2.828		1.000 11.22
ANISOU 1167 O GLU	156 1631	1199 1434	103 162 431
ATOM 1168 N PRO		20.158 41.118	1.000 10.29
ANISOU 1168 N PRO ATOM 1169 CD PRO	157 1329	1201 1381	-109 21 1 2 3
ATOM 1169 CD PRO ANISOU 1169 CD PRO	157 3.527 157 1381	21.407 40.359 1093 1391	1.000 10.17
ATOM 1170 CA PRO	157 3.618	20.363 42.553	1.000 10.28
ANISOU 1170 CA PRO	157 1160	1354 1391	-12 -61 6 4
ATOM 1171 CB PRO		21.805 42.590	1.000 12.44
ANISOU 1171 CB PRO		1567 1330	-397 20 5 8
ATOM 1172 CG PRO	157 3.475	22.471 41.429	1.000 10.44
ANISOU 1172 CG PRO	157 1469	1259 1237	-388 166 -15
ATOM 1173 C PRO ANISOU 1173 C PRO	157 2.387 157 1206	20.269 43.450 1554 1357	1.000 10.83 -89 -61 7 6
ATOM 1174 0 PRO	157 1.247	1554 1357 20.422 42.992	1.000 11.38
ANISOU 1174 O PRO	157 1157	1742 1426	-93 -64 3 3
ATOM 1175 N LEU	158 2.561	19.988 44.742	1.000 9.91
ANISOU 1175 N LEU	158 1011	1308 1447	-86 -53 151
ATOM 1176 CA LEU	158 1.524	19.940 45.764	1.000 10.85
ANISOU 1176 CA LEU	158 1319	1461 1344	-387 -2 -3
ATOM 1177 CB LEU ANISOU 1177 CB LEU	158 1.152	18.482 46.078	1.000 11.03 -251 99 9 3
ANISOU 1177 CB LEU ATOM 1178 CG LEU	158 1280 158 0.111	1447 1464 18.239 47.155	-251 99 9 3 1.000 12.01
ANISOU 1178 CG LEU	158 1271	1497 1795	-303 241 128
ATOM 1179 CD1 LEU	158 -1.212	18.826 46.736	1.000 16.21
ANISOU 1179 CD1 LEU	158 1224	2249 2685	-111 41 -239
ATOM 1180 CD2 LEU	158 -0.086	16.736 47.397	1.000 17.17
ANISOU 1180 CD2 LEU	158 2656	1542 2325	-254 1273 1 7 4
ATOM 1181 C LEU	158 1.997	20.626 47.048	1.000 11.22
ANISOU 1181 C LEU ATOM 1182 O LEU	158 1496 158 3.056	1366 1402 20.201 47.539	110 -304 5 1.000 11.28
ANISOU 1182 O LEU	158 1283	1368 1635	20 -262 7 5
ATOM 1183 N LEU	159 1.234	21.599 47.548	1.000 10.86
ANISOU 1183 N LEU	159 1103	1744 1278	68 - 180 - 70
ATOM 1184 CA LEU	159 1.540	22.278 48.797	
ANISOU 1184 CA LEU		1761 1407	
ATOM 1185 CB LEU			1.000 12.44
ANISOU 1185 CB LEU			-209 -73 -33
ATOM 1186 CG LEU ANISOU 1186 CG LEU			246 -54 -215
ATOM 1187 CD1 LEU		24.435 50.651	
ANISOU 1187 CD1 LEU			177 -292 1 0 4
ATOM 1188 CD2 LEU	159 1.442	26.134 49.640	
ANISOU 1188 CD2 LEU	159 1802	1721 1543	87 -87 - 20
ATOM 1189 C LEU		21.846 49.868	
ANISOU 1189 C LEU			
ATOM 1190 O LET	107 -0.000	21.940 49.620	T.000 T3.70

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- 129 -ANISOU 1190 O 159 1354 LEU 2395 -328 34 - 2691457 MOTA 1191 N ARG 160 1.013 51.010 21.385 1.000 14.59 ANISOU 1191 N ARG 160 1737 2569 1239 -390 -128 - 224 1192 CA ATOM ARG 21.030 160 0.158 52.153 1.000 13.94 ANISOU 1192 CA ARG 160 1265 2631 1402 157 -137921193 CB ATOM ARG 160 0.161 19.528 52.343 1.000 18.20 ANISOU 1193 CB ARG 2645 160 1932 2338 -301 32 1 9 3 ATOM 1194 CG ARG 160 -0.423 18.661 51.252 1.000 25.12 ANISOU 1194 CG ARG 160 3451 2902 3191 -653 -78723ATOM 1195 CD **ARG** 160 -0.765 51.831 1.000 31.98 17.301 ANISOU 1195 CD ARG 160 4825 3598 3729 -1994 -905 3.2 1 1196 NE MOTA ARG 16.322 160 -1.284 50.896 1.000 26.15 ANISOU 1196 NE ARG 160 3392 3587 2957 -739 -1056 3 1 0 1197 CZ ATOM ARG 160 -0.970 50.779 1.000 25.30 15.044 ANISOU 1197 CZ ARG 160 3195 3390 3028 94 - 785 295 1198 NH1 ARG MOTA 160 -0.063 14.433 51.552 1.000 31.26 ANISOU 1198 NH1 ARG 160 3654 4142 4080 -629 -1089 2054 1199 NH2 ARG ATOM 160 -1.572 14.308 49.850 1.000 28.82 ANISOU 1199 NH2 ARG 160 4020 3122 3807 -13 -966 - 901200 C ATOM ARG 160 0.649 53.447 21.669 1.000 15.12 ANISOU 1200 C 160 1649 ARG 2863 1232 104 -66 125 1201 0 ATOM ARG 160 1.804 21.556 53.863 1.000 17.09 ANISOU 1201 O ARG 160 1291 3411 1791  $-400 \quad 74 \quad -812$ ATOM 1202 N PHE 22.369 161 -0.258 54.114 1.000 14.95 ANISOU 1202 N 2506 PHE 161 1512 1660 -253 -8 -146 1203 CA ATOM 161 -0.036 PHE 22.949 55.427 1.000 13.27 ANISOU 1203 CA PHE 161 1600 1760 . 1681 -9 - 249- 4 1 1204 CB ATOM 24.381 PHE 161 -0.587 55.472 1.000 16.82 ANISOU 1204 CB PHE 161 1594 1947 2851 384 58 6 4 1205 CG ATOM PHE 25.109 161 - 0.31756.771 1.000 22.56 ANISOU 1205 CG PHE 161 2464 3684 2424 790 -1067 -39 1206 CD1 PHE ATOM 161 -1.175 25.010 57.849 1.000 26.03 ANISOU 1206 CD1 PHE 3620 161 3353 2919 267 1106 - 702 1207 CD2 PHE ATOM 161 0.822 56.885 25.901 1.000 25.34 ANISOU 1207 CD2 PHE 161 2353 3265 4011 -179 - 161 - 7381208 CE1 PHE ATOM 25.660 161 -0.943 59.051 1.000 30.50 ANISOU 1208 CE1 PHE 161 4784 3324 3481 -972 1456 - 620 1209 CE2 PHE ATOM 161 1.061 26.553 58.080 1.000 26.10 ANISOU 1209 CE2 PHE 161 2546 3067 -129 281 -1127 4302 1210 CZ ATOM PHE 161 0.199 26.438 59.164 1.000 30.06 ANISOU 1210 CZ 161 3839 PHE 3197 4386 -15.2 774 - 677 ATOM 1211 C PHE 56.447 1.000 13.93 161 - 0.73722.073 ANISOU 1211 C PHE 161 1842 1946 1503  $-334^{\circ}$  -277 -240ATOM 1212 0 PHE 161 -1.916 21.843 56.270 1.000 18.26 ANISOU 1212 O PHE 161 2000 3277 1662 -744 - 3994.75ATOM 1213 N ARG 162 -0.090 21.631 57.503 1.000 16.29 ANISOU 1213 N ARG 162 2063 2516 -937 -523 7 7 1610 1214 CA ATOM ARG 162 -0.635 20.719 58.483 1.000 15.62 ANISOU 1214 CA ARG 162 1772 2512 1650 -519 -266 7 6 1215 C ATOM ARG 162 - 0.47621.312 59.890 1.000 17.48 ANISOU 1215 C ARG 162 1855 3131 1656 -603 -186 - 76 ATOM 1216 0 ARG 162 0.609 21.734 60.251 1.000 17.23 ANISOU 1216 O ARG 162 1928 3063 1557 -771 - 42 - 1601217 CB ATOM 162 0.081 ARG 58.458 1.000 21.99 19.374 ANISOU 1217 CB ARG 162 3309 2318 -272 -737 - 22 2727 MOTA 1218 CG 162 -0.573 ARG 59.348 1.000 26.07 18.322 ANISOU 1218 CG 2375 ARG 162 3488 4041 489 655 280 1219 CD ATOM ARG 162 -0.231 58.886 1.000 25.85 16.896 ANISOU 1219 CD ARG 162 3106 2221 4495 418 -2 2 3 9 1220 NE ATOM 162 -0.943 15.916 59.698 1.000 28.83 ARG ANISOU 1220 NE 162 4379 ARG 2437 4139 -181 332 - 177

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14.638 59.879 1.000 27.99
ATOM
       1221 CZ
                ARG
                     162 -0.642
                     162 4271
ANISOU 1221 CZ
                                                -179
                ARG
                                 2497
                                         3868
                                                      962 8 4
                                 14.119 59.273 1.000 26.61
       1222 NH1 ARG
                     162 0.429
ATOM
ANISOU 1222 NH1 ARG
                     162 3200
                                 3167
                                         3742
                                                -91
                                                      -126 - 268
       1223 NH2 ARG
                     162 -1.408
                                 13.883 60.658 1.000 34.20
ATOM
ANISOU 1223 NH2 ARG
                     162 3807
                                 3522
                                         5663
                                                -986 702 780
       1224 N
MOTA
                TYR
                     163 -1.570
                                 21.296 60.622 1.000 16.77
ANISOU 1224 N
                TYR
                     163 1803
                                 2865
                                         1705
                                                -484 -194 8 4
                                 21.749 61.997 1.000 16.73
       1225 CA
                TYR
MOTA
                     163 -1.627
ANISOU 1225 CA
                TYR
                     163 1819
                                 2770
                                                -692 -51 4 0
                                         1766
       1226 CB
                                 22.804 62.116 1.000 18.99
                TYR
ATOM
                     163 -2.712
ANISOU 1226 CB
                TYR
                     163 2479
                                 2560
                                         2175
                                                 -427 -303 -214
                     163 -3.173
       1227 CG
ATOM
                TYR
                                 23.206 63.488 1.000 23.52
ANISOU 1227 CG
                     163 2573
                                 3821
                TYR
                                         2544
                                                 -16
                                                      -335 - 868
                                 23.848 64.367 1.000 31.80
       1228 CD1 TYR
                     163 -2.316
ATOM
ANISOU 1228 CD1 TYR
                     163 3613
                                 5005
                                         3466
                                                 -1151 304 -2338
       1229 CE1 TYR
                     163 -2.731
                                 24.222 65.625 1.000 40.74
ATOM
ANISOU 1229 CE1 TYR
                     163 5855
                                 5676
                                         3950
                                                 -1906 976 -3116
       1230 CD2 TYR
                     163 - 4.459
                                 22.965 63.931 1.000 32.55
ATOM
ANISOU 1230 CD2 TYR
                     163 3307
                                                -1066 639 -2340
                                 5654
                                         3408
       1231 CE2 TYR
                     163 -4.902
                                 23.332 65.189 1.000 42.99
ATOM
                                 6630
ANISOU 1231 CE2 TYR
                     163 5626
                                         4080
                                                -2352 1989 - 2949
       1232 CZ
                                 23.960 66.025 1.000 42.52
ATOM
                     163 -4.017
                TYR
                     163 6281
ANISOU 1232 CZ
                                 5799
                TYR
                                         4075
                                                 -1721 1943 - 3714
       1233 OH
                     163 -4.380
                                 24.351 67.274 1.000 48.87
ATOM
                TYR
ANISOU 1233 OH
                                         3569
                TYR
                     163 8167
                                 6831
                                                -269 1801 - 3052
       1234 C
ATOM
                TYR
                     163 -1.935
                                 20.551 62.896 1.000 17.90
ANISOU 1234 C
                TYR
                     163 2872
                                 2353
                                         1575
                                                 -894 -465 - 173
       1235 0
MOTA
                TYR
                     163 - 2.933
                                 19.858 62.653 1.000 18.12
ANISOU 1235 O
                                 2130
                TYR
                     163 2694
                                         2060
                                                 -732 -615 6 7
       1236 N
                PHE
                     164 -1.112
ATOM
                                 20.326 63.898 1.000 18.32
ANISOU 1236 N
                                 2621
                                         1826
                                                 -614 - 402 - 90
                PHE
                     164 2516
                PHE
ATOM
       1237 CA
                                 19.381 64.984 1.000 23.44
                     164 -1.340
ANISOU 1237 CA
                PHE
                     164 4176
                                 2692
                                         2038
                                                 -727 -669 2 1 9
       1238 CB
                                 18.617 65.327 1.000 26.02
ATOM
                PHE
                     164 -0.073
ANISOU 1238 CB
                                 2824
                PHE
                     164 4594
                                                 -459 -822 3 7 9
                                         2470
       1239 CG
                PHE
                     164 0.407
ATOM
                                 17.669 64.231 1.000 29.00
ANISOU 1239 CG
                PHE
                                 3639
                                                 -518 -427 -254
                     164 4118
                                         3263
       1240 CD1 PHE
                     164 1.224
ATOM
                                 18.118 63.205 1.000 27.11
ANISOU 1240 CD1 PHE
                     164 3040
                                 4013
                                         3249
                                                 -198 -821 4
ATOM 1241 CD2 PHE 164 0.051 16.332 64.240 1.000 28.37
ANISOU 1241 CD2 PHE
                     164 3935
                                 3139
                                         3704
                                                       30 - 64
                                                 472
       1242 CE1 PHE
                     164 1.657
                                 17.248 62.223 1.000 28.13
ATOM
ANISOU 1242 CE1 PHE
                                 3926
                     164 2730
                                         4034
                                                 -43 -229 6
                                 15.464 63.250 1.000 31.71
       1243 CE2 PHE
                     164 0.459
ATOM
                                                 -293 657 -383
ANISOU 1243 CE2 PHE
                                 3694
                                         3635
                     164 4719
ATOM
       1244 CZ
                PHE
                     164 1.276
                                 15.924 62.234 1.000 30.26
ANISOU 1244 CZ
                PHE
                     164 3827
                                  3808
                                         3862
                                                 0 300 1 2 6
                                20.160 66.228 1.000 24.65
ATOM
       1245 C
                 PHE
                     164 - 1.775
ANISOU 1245 C
                PHE
                     164 3541
                                  4049
                                         1777
                                                 -1025 -455 3 7
       1246 O
 MOTA
                 PHE
                     164 -0.889 20.713 66.885 1.000 25.54
ANISOU 1246 O
                 PHE
                                                 -921 -440 -257
                                         2019
                     164 3520
                                  4167
                     165 -3.058 20.293 66.527 1.000 32.24
       1247 N
 ATOM
                 PRO
                                                 -1894 266 -680
 ANISOU 1247 N
                 PRO
                     165 3641
                                  5095
                                         3513
       1248 CA
 ATOM
                 PRO
                     165 -3.486 21.012 67.720 1.000 32.98
 ANISOU 1248 CA
                                                 -1271 397 - 322
                 PRO
                      165 3570
                                  5737
                                         3225
       1249 C
                     165 -2.854 20.429 68.986 1.000 38.48
 ATOM
                 PRO
 ANISOU 1249 C
                 PRO
                     165 4355
                                  6808
                                         3457
                                                 -1872 40 3 4 3
        1250 O
 ATOM
                 PRO
                     165 -2.551 19.230 69.034 1.000 53.87
 ANISOU 1250 O
                 PRO
                     165 9948
                                 7012
                                          3507
                                                 -959 692 1750
 ATOM
        1251 CB
                PRO
                     165 -5.001 20.820 67.769 1.000 37.76
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ANISOU 1251 CB ATOM 1252 CG ANISOU 1252 CG ATOM 1253 CD ANISOU 1253 CD ATOM 1254 N ANISOU 1254 N ANISOU 1255 CA ANISOU 1255 CA ANISOU 1256 CB ANISOU 1256 CB ANISOU 1257 CG ANISOU 1257 CG ANISOU 1257 CG ANISOU 1258 CD1 ANISOU 1258 CD1 ANISOU 1259 CD2 ATOM 1259 CD2 ANISOU 1259 CD2 ANISOU 1260 C ANISOU 1260 C ANISOU 1261 O ANISOU 1261 O ANISOU 1262 N ANISOU 1262 N ANISOU 1263 CA ANISOU 1264 C ANISOU 1264 C	LEU 178 2972 LEU 178 8.208 LEU 178 5303 LEU 178 3.885 LEU 178 2107 LEU 178 2.845 LEU 178 2407 ARG 179 4.128 ARG 179 3.231 ARG 179 1860	6449       3948         7       19.816       65.734         6296       3828         8.087       66.987         3338       5918         9.117       66.116         3170       4312         8.534       65.027         3245       4688         7.948       65.348         2950       4674         7.367       64.073         4524       4713         8.964       65.937         3695       6850         9.909       65.420         3534       4686         9.351       65.086         4624       8016         11.200       65.160         3437       4089         11.973       64.321         3289       4365	-518 -349 - 398 1.000 35.70 -1656 -5 - 604 1.000 36.23 -26 1216 1175 1.000 28.63 377 1344 4 0 1 1.000 30.08 760 752 - 620 1.000 29.43 667 371 - 979 1.000 32.13 586 810 - 790 1.000 41.71 356 -1656 - 1154 1.000 27.18 -175 1776 8 3 3 1.000 39.60 -1253 1290 2183 1.000 25.65 -216 878 7 4 1 1.000 25.04 69 641 1 5
ATOM 1265 O ANISOU 1265 O	ARG 179 2.295 ARG 179 2545	11.687 62.139 3242 5079	441 -332 - 256
ATOM 1266 CB	ARG 179 3.517	13.480 64.451	1.000 28.58
ANISOU 1266 CB ATOM 1267 CG	ARG 179 3980 ARG 179 2.936	$3317  3561 \\ 14.092  65.724$	-110 <b>-</b> 843 5 7
ANISOU 1267 CG	ARG 179 2.936 ARG 179 3817	3725 3862	57 - 957 - 372
ATOM 1268 CD	ARG 179 3.307		
ANISOU 1268 CD			90 -1514 - 338
ATOM 1269 NE ANISOU 1269 NE	ARG 179 2.925 ARG 179 7035		
ATOM 1270 CZ			153 -310 - 15 2 1 000 3 9 4 3
ANISOU 1270 CZ	ARG 179 8420	3029 3532	-479 580 400
ATOM 1271 NH1	ARG 179 3.213	18.286 66.331	
	ARG 179 11745	5 4676 6273 3 17.896 68.457	
ANISOU 1272 NH2	2 ARG 179 2.546 2 ARG 179 5661		275 -1463 -173
ATOM 1273 N	MET 180 4.455	11.099 62.424	1.000 21.43
ANISOU 1273 N		_ · · · <del>_</del> · · · <del>_</del>	
ATOM 1274 CA ANISOU 1274 CA		10.539 61.108	
ATOM 1275 C		1965 3315 2 9.482 61.182	
ANISOU 1275 C	MET 180 2251		
ATOM 1276 O	MET 180 6.894		7 1.000 18.52
ANISOU 1276 O ATOM 1277 CB	MET 180 2237		
ANISOU 1277 CB	MET 180 5.041 MET 180 2571	•	5 1.000 22.64 -197 -549 683
ATOM 1278 CG			
ANISOU 1278 CG	MET 180 3918		
ATOM 1279 SD ANISOU 1279 SD			
ATOM 1280 CE			
ANISOU 1280 CE			
ATOM 1281 N	ALA 181 5.46	7 8.295 60.68	0 1.000 16.99
ANISOU 1281 N	ALA 181 2144	2139 2174	-90 -558 2 9 9

- 132 -7.168 ATOM 1282 CA ALA181 6.396 60.676 1.000 16.12 ANISOU 1282 CA 1958 1890 -171 -343 6 0 2 ALA181 2275 1283 CB ALA 181 5.668 5.891 60.279 1.000 20.24 ATOM ANISOU 1283 CB 181 2857 2158 2673 -648 694 106 ALA 59.738 1.000 15.43 1284 C ALA 181 7.576 7.409 ATOM ANISOU 1284 C 181 2223 ALA 1717 1925 -315 -369 4 3 2 58.783 1.000 15.49 1285 0 181 7.458 ALA 8.198 ATOM ANISOU 1285 O ALA 181 2268 1761 1858 -173 -296 4 3 4 6.733 1286 N PRO ATOM 182 8.698 59.986 1.000 16.03 ANISOU 1286 N 182 2517 1745 1829 PRO 32 - 78 5 3 1 1287 CD PRO 182 8.983 5.802 ATOM 61.101 1.000 19.61 ANISOU 1287 CD PRO 182 2321 2908 2221 -210 -306 1 2 4 0 1288 CA PRO 182 9.865 6.907 MOTA 59.076 1.000 14.78 ANISOU 1288 CA 1336 182 2573 1706 PRO -101 -86 299 1289 CB PRO 182 10.914 5.948 59.649 1.000 16.20 ATOM ANISOU 1289 CB PRO 182 2570 1978 1607 170 -251771290 CG 182 10.479 5.713 61.066 1.000 19.28 PRO ATOM ANISOU 1290 CG PRO 182 2301 3071 1952 -199 -245 1 0 0 1 1291 C PRO 182 9.541 6.571 57.627 1.000 14.90 ATOM . ANISOU 1291 C PRO 1658 182 2230 1772 -421 - 2623401292 0 182 8.920 5.573 57.249 1.000 15.38 ATOM PRO -467 -482 5 3 9 ANISOU 1292 O PRO 182 2301 1587 1957 ATOM 1293 N 56.730 183 9.969 7.460 1.000 12.28 HIS ANISOU 1293 N HIS 1617 183 1737 1312 -154 - 284 1 5 67.354 183 9.733 55.300 1.000 11.90 ATOM 1294 CA HIS -254 -351 3 5 ANISOU 1294 CA HIS 183 1413 1495 1614 1295 CB ATOM HIS 183 8.300 7.824 54.922 1.000 12.43 ANISOU 1295 CB HIS 1368 1957 -128 -241 1 1 2 183 1399 1296 CG HIS 183 8.168 9.314 55.089 1.000 11.36 ATOM -367 -296 5 6 ANISOU 1296 CG HIS 1369 183 1349 1600 1297 CD2 HIS 183 8.259 10.374 54.249 1.000 12.03 MOTA 1589 ANISOU 1297 CD2 HIS 1296 -43 157 - 10183 1684 1298 ND1 HIS 56.339 1.000 13.27 183 7.989 9.858 ATOM ANISOU 1298 ND1 HIS 267 193 1439 183 1901 1700 -65 1299 CE1 HIS ATOM 183 7.943 11.187 56.244 1.000 12.43 ANISOU 1299 CE1 HIS 183 1939 1490 1296 77 -244 150 11.515 1300 NE2 HIS 183 8.101 54.992 1.000 11.04 ATOM ANISOU 1300 NE2 HIS 183 1560 1437 1199 215 -232 4 8 ATOM 1301 C HIS 183 10.749 8.176 54.515 1.000 12.27 -303 -282 - 67ANISOU 1301 C HIS 183 1446 1577 1639 9.032 ATOM 1302 O HIS 183 11.433 55.064 1.000 12.94 ANISOU 1302 O 183 1496 1915 1505 -558 -292 1 5 HIS TYR 184 10.849 ATOM 1303 N 7.907 53.215 1.000 10.61 ANISOU 1303 N TYR 184 1453 1027 1552 -41 -380110184 11.483 52.256 1.000 11.36 TYR 8.800 ATOM 1304 CA ANISOU 1304 CA TYR 1104 -264178184 1475 1738 -71 1305 CB TYR 184 12.628 8.151 51.481 1.000 11.79 MOTA ANISOU 1305 CB TYR 184 1631 1114 1734 -62 -197346.907 50.677 1.000 11.29 ATOM 1306 CG TYR 184 12.368 ANISOU 1306 CG 184 1680 921 1688 225 -893 174 TYR 51.268 1.000 11.76 184 12.156 5.659 ATOM 1307 CD1 TYR 927 1879 ANISOU 1307 CD1 TYR 184 1663 388 -487 190 ATOM 1308 CE1 TYR 184 11.911 4.526 50.492 1.000 12.64 878 1964 ANISOU 1308 CE1 TYR 184 1960 173 -40 182 MOTA 1309 CD2 TYR 184 12.333 6.949 49.279 1.000 11.13 ANISOU 1309 CD2 TYR 184 1252 1302 1674 109 -283 9 3 1310 CE2 TYR 48.502 1.000 12.93 ATOM 184 12.102 5.834 ANISOU 1310 CE2 TYR 1546 184 1944 1422 49 - 384 7 3 1311 CZ TYR 184 11.898 4.611 49.121 1.000 13.14 ATOM ANISOU 1311 CZ TYR 1304 30 -611 6 7 184 1717 1972 MOTA 1312 OH 184 11.663 3.490 48.343 1.000 15.45 TYR

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- 133 -ANISOU 1312 OH TYR 184 2028 1471 2373 42 - 476 - 247 1313 C 184 10.447 TYR ATOM 9.390 51.314 1.000 11.50 ANISOU 1313 C TYR 184 1445 1215 1709 -187 -201 3 4 8 1314 0 TYR ATOM 184 9.362 8.797 51.089 1.000 11.75 1853 ANISOU 1314 O TYR 184 1305 1308 -106 -171 4 2 7 1315 N ASP MOTA 185 10.784 50.743 1.000 10.79 10.557 ANISOU 1315 N ASP 185 1581 1069 1449 -141-132 1 1 8 185 9.861 1316 CA ASP MOTA 11.218 49.815 1.000 9.10 185 1089 ANISOU 1316 CA ASP 1093 1277 -326 23 2 0 6 1317 CB ASP 185 9.934 49.886 1.000 10.13 ATOM 12.743 ANISOU 1317 CB ASP 185 1427 1095 1327 -298 -178 1 7 7 1318 CG ASP 13.388 51.185 1.000 11.79 MOTA 185 9.540 ANISOU 1318 CG ASP 185 1797 1350 1333 -250 -149 1 1 1319 OD1 ASP 185 9.681 14.638 51.278 1.000 13.79 ATOM ANISOU 1319 OD1 ASP 185 2050 1316 1875 135 -52 - 26 1320 OD2 ASP ATOM 185 9.114 12.755 52.189 1.000 13.31 ANISOU 1320 OD2 ASP 185 1805 1848 1405 -411 -63 105 1321 C ASP ATOM 185 10.098 10.759 48.371 1.000 9 . 4 4 ANISOU 1321 C ASP 185 1036 1150 1401 -309 -26 100 1322 0 ASP ATOM 185 11.234 10.469 48.005 1.000 10.64 ANISOU 1322 O ASP 185 1167 1376 1500 -127 -35 -2061323 N 186 9.038 LEU ATOM 10.684 47.568 1.000 10.09 186 1211 ANISOU 1323 N LEU 1186 1437 -272 -177 - 58 ATOM LEU 1324 CA 186 9.124 10.312 46.161 1.000 10.60 ANISOU 1324 CA LEU 186 1641 986 1401 -239 -52 -441325 CB LEU 9.295 ATOM 186 8.030 45.798 1.000 11.32 ANISOU 1325 CB LEU 186 1652 929 1721 -111 17 - 479 1326 CG LEU 186 7.989 ATOM 7.977 46.602 1.000 12.60 ANISOU 1326 CG LEU 186 1408 1039 2340 -263 -200 - 166 1327 CD1 LEU ATOM 186 6.896 7.064 46.028 1.000 16.64 ANISOU 1327 CD1 LEU 186 1900 1373 3049 -634 -398 -135 1328 CD2 LEU 186 9.356 ATOM 7.332 46.629 1.000 13.84 ANISOU 1328 CD2 LEU 186 1438 1245 2575 -155 443 283 1329 C 186 9.024 ATOM LEU 1.000 10.90 11.521 45.223 ANISOU 1329 C LEU 186 1327 1211 1603 -3 -451 164 1330 0 MOTA LEU 186 8.768 11.406 44.031 1.000 13.60 ANISOU 1330 O 186 2067 LEU 1608 1494 -211 -321 1 0 3 ATOM 1331 N SER 187 9.264 12.705 45.734 1.000 10.71 ANISOU 1331 N SER 187 1546 1129 1393 -76 -282 3 1 8 ATOM 1332 CA SER 187 9.401 13.943 44.998 1.000 10.49 ANISOU 1332 CA SER 187 1427 1191 1370 195 -10748815.103 46.002 1.000 10.56 187 9.221 ATOM 1333 CB SER ANISOU 1333 CB SER 187 1105 1857 298 161 532 1048 1334 OG 14.918 46.726 1.000 13.01 ATOM SER 187 10.430 ANISOU 1334 OG SER 187 1343 2169 -132 -295 2 0 1 1432 1335 C ATOM SER 187 10.774 14.062 44.336 1.000 10.47 ANISOU 1335 C SER 187 1447 135 862 1669 -3 1 4 5 1336 0 ATOM SER 13.246 44.513 1.000 10.54 187 11.684 ANISOU 1336 O SER 187 1577 799 1629 183 -91 - 771337 N ATOM MET 188 10.962 15.095 43.502 1.000 9 . 7 8 ANISOU 1337 N MET 188 1419 978 1318 147 44 7 4 MOTA 1338 CA MET 188 12.267 15.584 43.065 1.000 9 . 9 4 ANISOU 1338 CA MET 188 1394 942 1441 182 58 3 7 MOTA 1339 CB MET 188 12.128 16.543 41.891 1.000 10.89 ANISOU 1339 CB 188 1523 MET 840 1774 98 48 2 2 7 MOTA 1340 CG MET 17.258 41.470 1.000 11.40 188 13.385 ANISOU 1340 CG MET 188 1403 1172 1756 46 -51 2 1 4 ATOM 1341 SD MET 16.134 40.891 1.000 12.71 188 14.687 ANISOU 1341 SD MET 188 1619 1272 139 137 198 1940 1342 CE 188 16.061 17.267 40.790 1.000 13.86 ATOM MET ANISOU 1342 CE MET 188 1862 1399 -2 911 - 9 0 2003

- 134 -ATOM 1343 C MET 16.217 44.291 1.000 12.13 188 12.946 ANISOU 1343 C MET 1586 188 1325 169 1698 -18 - 2851344 0 ATOM MET 188 13.971 15.727 44.804 1.000 11.52 ANISOU 1344 O MET 188 1288 1553 1535 144 132 8 7 ATOM 1345 N 189 12.362 17.290 44.838 1.000 10.00 VAL ANISOU 1345 N VAL 1292 53 -175 6 189 1290 1217 189 12.745 ATOM 1346 CA 46.099 1.000 9.70 VAL 17.894 ANISOU 1346 CA VAL 189 1209 1057 1420 -212 - 45 - 19ATOM 1347 CB VAL 189 13.618 19.154 45.979 1.000 9 . 9 7 ANISOU 1347 CB VAL 1398 189 1288 1103 -238 129 189 1348 CG1 VAL 45.266 1.000 13.45 ATOM 189 14.953 18.837 ANISOU 1348 CG1 VAL 189 1334 1410 2368 -236 390 143 ATOM 1349 CG2 VAL 189 12.899 45.264 1.000 12.24 20.289 ANISOU 1349 CG2 VAL 189 1715 1242 -25 1693 150 295 ATOM 1350 C VAL 18.245 46.871 1.000 10.10 189 11.469 189 1089 ANISOU 1350 C VAL 1600 1149 -456 -156 -73ATOM 1351 0 VAL 189 10.405 18.399 46.250 1.000 9.53 ANISOU 1351 O VAL 189 1153 1249 1217 -222 -190 8 1352 N ATOM THR 190 11.609 18.327 48.187 1.000 8.66 ANISOU 1352 N 15 -202 127 THR 894 1123 190 1273 1353 CA 18.771 49.091 1.000 9.64 ATOM THR 190 10.565 ANISOU 1353 CA THR 190 1350 1167 1147 -11 -228 - 991354 CB 17.699 ATOM 190 10.194 THR 50.132 1.000 10.69 ANISOU 1354 CB THR 190 1231 1196 1635 -300 121 - 541355 OG1 THR MOTA 190 9.662 16.586 49.501 1.000 12.45 ANISOU 1355 OG1 THR 190 1333 1341 2055 -140 -258 - 481356 CG2 THR 190 9.038 ATOM 51.019 1.000 13.59 18.131 ANISOU 1356 CG2 THR 190 1121 2222 1821 -272 151 -195ATOM 1357 C THR 190 11.058 19.976 49.891 1.000 9.23 ANISOU 1357 C THR 190 1257 **-1**02 **-3**36 **-**49 1096 1152 ATOM 1358 0 50.447 1.000 10.54 190 12.149 THR 19.867 ANISOU 1358 O 190 1322 1292 THR 1390 -5 -359 -122 ATOM 1359 N LEU 191 10.313 21.064 49.978 1.000 10.23 ANISOU 1359 N LEU 191 1319 1167 1401 -71 -177 - 133ATOM 1360 CA LEU 191 10.691 22.241 50.770 1.000 10.19 ANISOU 1360 CA LEU 1176. 191 1259 1438 0 - 294 - 1421361 CB ATOM LEU 191 10.604 23.511 49.910 1.000 11.52 ANISOU 1361 CB LEU 191 1203 1185 1990 -118 -601 3 2 23.898 49.167 1.000 13.23 LEU MOTA 1362 CG 191 11.897 ANISOU 1362 CG LEU 191 1898 1710 1419 -391 -358 9 7 ATOM 1363 CD1 LEU 191 12.333 22.794 48.218 1.000 15.25 ANISOU 1363 CD1 LEU 191 1685 2018 2091 -476 -214 -3051364 CD2 LEU 191 11.717 25.231 48.448 1.000 17.46 ATOM ANISOU 1364 CD2 LEU 191 2310 2044 2281 -14 17 6 0 4 1365 C 191 9.798 22.328 52.006 1.000 11.93 ATOM LEU ANISOU 1365 C LEU 56 - 190 - 372 191 1275 1677 1579 ATOM 1366 0 LEU 22.262 51.868 1.000 13.49 191 8.560 ANISOU 1366 O LEU 191 1276 2173 1676 1 -192 -601 ATOM ILE 22.483 53.190 1.000 11.06 1367 N 192 10.394 ANISOU 1367 N ILE 192 1115 1603 1487 -111 -92 -108 1368 CA MOTA ILE 192 9.671 22.539 54.443 1.000 11.13 ANISOU 1368 CA 192 1071 ILE 1638 .1521 11 -173 -149 1369 CB ILE MOTA 21.304 55.330 1.000 12.94 192 9.927 ANISOU 1369 CB ILE 192 2099 1232 1586 -65 -9 -2331370 CG2 ILE ATOM 192 9.221 21.428 56.673 1.000 16.06 ANISOU 1370 CG2 ILE 192 2479 1983 1641 - -206 426 - 215 1371 CG1 ILE 192 9.512 ATOM 20.028 54.590 1.000 15.51 ANISOU 1371 CG1 ILE 192 2633 1658 1601 -400 - 48 - 1751372 CD1 ILE 192 9.845 ATOM 18.765 55.339 1.000 25.71 ANISOU 1372 CD1 ILE 192 5869 1608 2290 -175 -1566 -301 1373 C ATOM ILE 192 9.966 23.809 55.253 1.000 11.47

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ANISOU	1373	C	ILE	192	1330	1603	1427	4 222 122
ATOM	1374	O	ILE		11.123			-4 -222 -122
						24.106	55.567	1.000 13.33
ANISOU	1374	0	ILE		1344	1738	1981	-96 -289 - 219
ATOM	1375	N	${ t GLN}$	193	8.904	24.525	55.602	1.000 15.78
ANISOU	1375	N	GLN		1316	2462	2219	
ATOM	1376		GLN					-64 -5 -975
					8.987	25.653	56.533	1.000 14.56
ANISOU	1376		GLN	193	1582	1858	2091	212 -304 - 529
$\mathtt{ATOM}$	1377	CB	${ t GLN}$	193	8.449	26.975	56.020	1.000 20.03
ANISOU	1377	CB	GLN	193	2226	2203	3180	· · · = <del>-</del>
ATOM	1378	CG	GLN		9.203			318 -329 1 4 2
					· · · · ·	27.684	54.914	1.000 23.86
ANISOU	1378	CG	GLN		3399	2492	3174	313 45 2 8 0
ATOM	1379	CD	GLN	193	8.665	29.079	54.675	1.000 22.92
ANISOU	1379	CD	GLN	193	3250	2363	3097	78 - 477 2 0 5
ATOM	1380	OE1	GLN	193	7.603	29.292	54.099	
ANISOU		OE1			4175			1.000 27.68
						3310	3031	552 -1214 2 9
ATOM	1381	NE2		193	9.411	30.075	55.134	1.000 27.01
	1381	NE2	GLN	193	3187	2667	4408	-440 124 1 7
ATOM	1382	С	GLN	193	8.216	25.265	57.804	1.000 15.14
ANISOU	1382	C	GLN		1945	1827	1982	
ATOM	1383	Ō	GLN		7.147			136 -174 - 722
ANISOU						24.662	57.714	1.000 27.80
	1383	0	GLN		2523	6225	1817	-1586 -592 2 3 5
MOTA	1384	N	GLN	194	8.714	25.552	58.978	1.000 19.80
ANISOU	1384	N	GLN	194	2994	2502	2025	-632 -752 3 3
ATOM	1385	CA	GLN		8.100	25.080		1.000 22.89
ANISOU			GLN		3961			
ATOM	1386					2626	2110	493 -20 5 2
			GLN		7.763		61.141	1.000 27.79
ANISOU			GLN		4886	2757	2916	823 25 - 262
ATOM	1387	0	GLN	194	8.424	27.258	60.983	1.000 30.03
ANISOU	1387	0	GLN		4727	3168	3516	368 -259 - 910
ATOM	1388		GLN		9.086			
ANISOU						_		1.000 23.97
			GLN		3952	3133	2021	846 483 352
ATOM	1389		GLN		9.398	22.835	60.314	1.000 21.94
ANISOU			GLN	194	2740	3238	2358	683 -182 - 1 0
ATOM	1390	CD	GLN	194	10.546	22.148		1.000 20.51
ANISOU			GLN		2450	3433	1911	
	1391							
					11.707	<b></b>		1.000 20.80
ANISOU			GLN		2245	2996		-171 -382 -681
ATOM	1392			194	10.223	21.585	62.197	1.000 24.91
ANISOU	1392	NE2	GLN	194	2539	3902	3023	210 -365 7 6 0
ATOM	1393	N	THR		6.817			1.000 32.47
ANISOU	1393	N	THR		5716			
ATOM	1394						3891	1095 1056 - 616
			THR		6.588	26.708	- <del>-</del> -	1.000 35.83
ANISOU			THR		6329	3539	3748	1011 999 - 722
ATOM	1395		THR	195	5.263	27.492	63.357	1.000 37.96
ANISOU	1395	CB	THR	195	5756	4304	4365	647 2095 - 1151
ATOM	1396	OG1	THR		4.191			1.000 48.36
ANISOU					6874	6076		
ATOM							5423	-806 2581 -1842
	1397				4.958			1.000 44.54
ANISOU					2944	7471	6510	-872 -963 6 2 1
ATOM	1398	С	THR	195	6.590	25.684	64.429	1.000 48.86
ANISOU	1398	С	THR		10133	4924		-321 -1356 - 221
ATOM	1399	0	THR		6.122	24.544		
ANISOU								1.000 64.12
			THR		13267	4150	6945	-264 -4541 1682
ATOM	1400		PHE		12.035	21.374	72.205	1.000 71.12
ANISOU			PHE	201	13961	9034	4028	-5932 -1658 -1741
ATOM	1401	CA	PHE	201	11.775	20.053		1.000 49.44
ANISOU	1401	CA	PHE		7918	7543	3326	-3128 1317 - 1488
ATOM	1402		PHE		10.469			
ANISOU						19.464		1.000 47.85
			PHE		7119	6892	4168	-1869 1937 -1899
ATOM	1403		PHE		10.130	18.113	71.545	1.000 46.41
ANISOU	1403	CG	PHE	201	6643	6596	4396	-2038 1879 -1497
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1404 CD1 PHE
ATOM
                      201 10.738
                                 16.954
                                        71.991 1.000 50.03
ANISOU 1404 CD1 PHE
                      201 7982
                                 6634
                                         4393
                                                -2326 1092 - 991
        1405 CD2 PHE
MOTA
                      201 9.220
                                 18.001
                                        70.513 1.000 42.63
ANISOU 1405 CD2 PHE
                      201 5458
                                 6427
                                         4313
                                                -1097 2449 -2268
        1406 CE1 PHE
                      201 10.434
ATOM
                                 15.739
                                        71.417 1.000 49.95
ANISOU 1406 CE1 PHE
                      201 8275
                                 6464
                                         4240
                                                -2047227 - 716
       1407 CE2 PHE
MOTA
                      201 8.901
                                 16.783 69.934 1.000 41.38
ANISOU 1407 CE2 PHE
                      201 6016
                                 5946
                                         3762
                                                -578 2006 - 1844
                      201 9.515
                PHE
ATOM
        1408 CZ
                                 15.636
                                        70.392 1.000 44.74
ANISOU 1408 CZ
                      201 7075
                PHE
                                         3663
                                 6261
                                                -1063 1020 - 975
                PHE
                                        70.107 1.000 42.42
ATOM
        1409 C
                      201 11.722
                                 20.110
ANISOU 1409 C
                PHE
                      201 6324
                                 6442
                                         3351
                                                -1964 717 -1441
                      201 11.007
                PHE
MOTA
        1410 0
                                 20.941 69.536 1.000 47.79
                PHE
ANISOU 1410 O
                      201 9668
                                 4400
                                         4090
                                                -762 691 -2416
                      202 12.477 19.232 69.449 1.000 34.04
       1411 N
ATOM
                VAL
ANISOU 1411 N
                VAL
                      202 4525
                                 5852
                                         2558
                                                -19487 - 425
        1412 CA
ATOM
                VAL
                      202 12.535
                                19.245 67.993 1.000 25.09
ANISOU 1412 CA
                      202 3221
                                 3752
                VAL
                                         2558
                                                -1041 -182 9 9
        1413 CB
                                 19.286 67.489 1.000 22.88
MOTA
                VAL
                      202 13.988
ANISOU 1413 CB
                VAL
                      202 2832
                                 3430
                                         2432
                                                -577 -691 -198
        1414 CG1 VAL
                                        65.965 1.000 26.02
                      202 14.053
ATOM
                                 19.387
ANISOU 1414 CG1 VAL
                      202 3821
                                         2470
                                 3594
                                                -958 \quad 35 \quad -277
        1415 CG2 VAL
                      202 14.771
                                        68.078 1.000 24.69
ATOM
                                 20.443
ANISOU 1415 CG2 VAL
                                 3473
                      202 3043
                                         2867
                                                -786 -410 -320
MOTA
        1416 C
                 VAL
                      202 11.798
                                 18.035
                                        67.421 1.000 20.69
ANISOU 1416 C
                 VAL
                                 2810
                                         2023
                      202 3027
                                                 -648 58 615
       1417 0
 ATOM
                      202 12.288
                 VAL
                                 16.914 67.581 1.000 26.08
ANISOU 1417 O
                 VAL
                      202 3294
                                  3219
                                         3396
                                                 -136 452 884
                      203 10.662
MOTA
        1418 N
                 SER
                                 18.234 66.766 1.000 20.21
ANISOU 1418 N
                 SER
                      203 3100
                                  2794
                                         1787
                                                 -414 25 -152
                      203 9.820
 ATOM
        1419 CA
                 SER
                                  17.192
                                         66.218 1.000 20.37
ANISOU 1419 CA
                 SER
                      203 3149
                                  2709
                                         1884
                                                 -355 129 -256
 ATOM
        1420 CB
                 SER
                      203 8.437
                                  17.779 65.896 1.000 24.72
 ANISOU 1420 CB
                 SER
                      203 2726
                                  4106
                                         2558
                                                 -178 369 -1015
 ATOM
        1421 OG
                 SER
                      203 7.841
                                  18.239
                                        67.097 1.000 31.80
 ANISOU 1421 OG
                 SER
                      203 3328
                                  5782
                                                 -457 1175 -1104
                                         2974
        1422 C
 ATOM
                 SER
                      203 10.367
                                  16.524 64.958 1.000 19.13
 ANISOU 1422 C
                 SER
                      203 2580
                                  2647
                                         2040
                                                 -339 170 -244
        1423 0
                      203 10.279
 ATOM
                 SER
                                 15.302 64.832 1.000 17.01
                     203 2311
                 SER
 ANISOU 1423 O
                                  2625
                                         1527
                                                 -414 206 - 18
 ATOM 1424 N
              LEU 204 10.902 17.259 63.998 1.000 16.16
 ANISOU 1424 N
                 LEU
                      204 2142
                                  1976
                                         2024
                                                 71.77 - 292
        1425 CA LEU
 ATOM
                      204 11.403 16.679 62.740 1.000 14.07
 ANISOU 1425 CA LEU
                                  1626
                      204 1670
                                         2049
                                                 -22 -24 -283
 ATOM
        1426 CB
                 LEU
                      204 11.269
                                  17.704 61.618 1.000 13.80
 ANISOU 1426 CB
                LEU
                      204 1549
                                  1763
                                         1931
                                                 -249 \quad -340 \quad -277
 ATOM
                                  17.272 60.212 1.000 14.13
        1427 CG
                 LEU
                      204 11.647
 ANISOU 1427 CG
                LEU
                      204 1726
                                  1722
                                                 -253 -482 -412
                                         1919
        1428 CD1 LEU
 ATOM
                      204 10.770 16.134 59.680 1.000 18.76
 ANISOU 1428 CD1 LEU
                      204 2579
                                  2895
                                         1654
                                                 -1297 -927 - 106
        1429 CD2 LEU
 ATOM
                      204 11.609 18.478 59.255 1.000 16.20
 ANISOU 1429 CD2 LEU
                      204 1987
                                  2095
                                         2074
                                                 6575 - 123
 ATOM
        1430 C
                 LEU
                      204 12.832
                                 16.140 62.885 1.000 14.81
 ANISOU 1430 C
                 LEU
                      204 1734
                                  1748
                                                 9 - 199 - 250
                                          2144
 ATOM
        1431 0
                 LEU
                      204 13.699 16.853 63.397 1.000 15.52
 ANISOU 1431 O
                 LEU
                      204 1833
                                  1789
                                         2274
                                                       -435 - 42
                                                 -59
        1432 N
 ATOM
                 GLN
                      205 13.065
                                 14.900 62.469 1.000 14.42
 ANISOU 1432 N
                 GLN
                      205 1847
                                  1804
                                          1827
                                                 189 -120 - 153
ATOM
        1433 CA
                 GLN
                      205 14.288 14.143 62.574 1.000 12.76
 ANISOU 1433 CA
                      205 1777
                 GLN
                                  1655
                                          1419
                                                 43 - 347 - 113
 ATOM
                      205 14.622 13.434 61.260 1.000 11.12
        1434 C
                 GLN
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- 138 -1465 0 ATOM 209 25.850 7.934 GLY60.991 1.000 35.98 ANISOU 1465 O 209 4448 3946 GLY 5279 1425 -426 1769 ATOM 1466 N 210 23.951 7.786 59.869 1.000 25.89 GLY GLY ANISOU 1466 N 210 3802 2756 3278 523 899 749 ATOM 1467 CA GLY 210 23.477 6.678 60.671 1.000 26.43 ANISOU 1467 CA GLY 3427 210 4479 2136 1228 742 912 GLY 62.016 1.000 28.45 ATOM 1468 C 210 22.885 7.025 ANISOU 1468 C GLY210 5472 2099 3237 831 1029 1175 1469 O GLY 62.789 1.000 40.26 ATOM 210 22.634 6.098 ANISOU 1469 O 2719 210 7322 GLY 5256 1881 2759 2360 211 22.651 ATOM 1470 N 8.281 62.338 1.000 25.78 ALA ANISOU 1470 N ALA 211 4671 2359 2763 1370 724 1197 1471 CA 211 22.048 ATOM 63.613 1.000 23.74 ALA8.671 ANISOU 1471 CA 211 2966 2896 ALA3156 727 339 663 1472 CB ALA 64.496 1.000 29.57 ATOM 211 23.093 9.333 ANISOU 1472 CB ALA 211 2957 4372 3906 834 -96 6 9 ATOM 1473 C ALA 63.360 1.000 21.19 211 20.900 9.626 ANISOU 1473 C ALA 211 3090 2611 2350 484 178 741 1474 0 ATOM 10.381 62.399 1.000 23.91 211 20.936 ALA ANISOU 1474 O 211 3771 2653 ALA 2659 -30 -66 930 1475 N ATOM 212 19.889 9.629 PHE 64.204 1.000 19.88 ANISOU 1475 N 212 2603 PHE 2577 2375 398 -128 3 7 4 212 18.814 10.613 64.130 1.000 19.13 1476 CA PHE ATOM ANISOU 1476 CA PHE 212 2581 2257 2432 284 -565 3 1 7 212 19.320 1477 C 12.006 64.489 1.000 20.00 PHE ATOM ANISOU 1477 C PHE 212 3004 2480 2115 -640 6 8 133 212 19.893 12.230 65.569 1.000 21.10 MOTA 1478 O PHE ANISOU 1478 O PHE -391 212 2497 3558 1964 -406 2 2 2 10.290 65.096 1.000 21.37 MOTA 1479 CB PHE 212 17.688 ANISOU 1479 CB PHE 212 2553 2616 2952 293 -197 - 1841480 CG PHE ATOM 212 17.010 8.950 64.912 1.000 23.4<sup>-</sup>5 ANISOU 1480 CG PHE 212 2161 3496 3253 -376 -282 -5581481 CD1 PHE 212 16.369 65.990 1.000 23.33 ATOM 8.377 ANISOU 1481 CD1 PHE 212 2545 3115 -382 -350 - 508 3206 212 17.029 ATOM 1482 CD2 PHE 8.302 63.687 1.000 25.83 ANISOU 1482 CD2 PHE 3962. 212 2554 -622 -217 -7873299 1483 CE1 PHE ATOM 212 15.730 7.149 65.872 1.000 28.13 212 3784 ANISOU 1483 CE1 PHE -1119 96 - 973 3544 3362 1484 CE2 PHE MOTA 212 16.419 7.072 63.569 1.000 23.04 ANISOU 1484 CE2 PHE 212 2504 3289 382 2960 -232 - 558ATOM 1485 CZ PHE 212 15.781 6.486 64.651 1.000 27.88 ANISOU 1485 CZ PHE 212 3658 3977 2957 -1072 -501 - 760 1486 N THR 213 19.076 12.936 63.578 1.000 18.30 ATOM THR 213 2690 ANISOU 1486 N 2083 2181 149 -583 - 93 1487 CA THR 213 19.566 14.310 63.681 1.000 17.99 MOTA ANISOU 1487 CA THR 213 1976 2139 2721 230 -686 - 287 213 20.515 14.586 62.498 1.000 20.43 ATOM THR 1488 CB ANISOU 1488 CB THR: 213 1798 3683 2280 140 - 119 - 4231489 OG1 THR 213 21.638 13.695 62.629 1.000 25.33 ATOM ANISOU 1489 OG1 THR 213 2571 3378 3676 925 71 5 2 8 1490 CG2 THR 213 21.087 15.985 62.485 1.000 21.11 ATOM ANISOU 1490 CG2 THR 213 1935 -310 -289 -747. 2667 3420 ATOM 1491 C 213 18.391 15.277 63.641 1.000 15.53 THR ANISOU 1491 C 111 -557 - 167 THR 213 1732 2135 2032 213 17.533 15.195 62.761 1.000 16.11 MOTA 1492 0 THR ANISOU 1492 O THR 213 1742 2197 2180 -327 -669 5 6 214 18.362 16.199 64.590 1.000 15.60 ATOM 1493 N ASP ANISOU 1493 N ASP 214 2025 2046 1857 64 - 405 2 1494 CA ASP 214 17.380 17.256 64.672 1.000 15.59 ATOM ANISOU 1494 CA ASP 214 2130 1722 2072 2 -1010 - 242 214 17.744 18.200 65.822 1.000 17.13 ATOM ASP 1495 CB

- 139 -ANISOU 1495 CB ASP 214 2528 1893 2086 -226 -1022 -247 1496 CG ATOM ASP 214 17.612 17.672 67.219 1.000 20.21 ANISOU 1496 CG ASP 214 3138 2495 2045 -451 -1276 - 1481497 OD1 ASP MOTA 214 17.079 16.571 67.460 1.000 20.87 ANISOU 1497 OD1 ASP 214 2778 2632 2518 -505 1 5 1 -247 1498 OD2 ASP MOTA 214 18.076 18.401 68.127 1.000 28.05 ANISOU 1498 OD2 ASP 214 5110 3118 2429 -257 -1997 - 6191499 C ASP MOTA 214 17.314 18.146 63.441 1.000 15.14 ASP ANISOU 1499 C 214 2029 1822 1901 -574 - 319182 1500 O ATOM ASP 214 18.349 18.552 1.000 17.63 62.897 ANISOU 1500 O ASP 214 1956 2032 2710 -214 -810 - 151501 N ATOM LEU 215 16.105 18.493 63.027 1.000 14.69 ANISOU 1501 N 1758 LEU 215 1936 1887 38 -334 2 4 2 ATOM 1502 CA LEU 215 15.915 19.504 61.979 1.000 13.35 ANISOU 1502 CA LEU 215 1820 1753 1498 89 - 22 5 9 ATOM 1503 CB LEU 215 15.352 18.819 60.734 1.000 14.24 ANISOU 1503 CB 215 1735 LEU 2167 1506 -98 75 - 31504 CG ATOM LEU 215 16.291 17.813 60.056 1.000 16.39 ANISOU 1504 CG LEU 2285 215 2031 1911 -340 320 - 424 1505 CD1 LEU ATOM 215 15.517 16.999 59.031 1.000 22.61 ANISOU 1505 CD1 LEU 215 3139 2024 3427 -801 -877 -10 1506 CD2 LEU 215 17.482 ATOM 18.543 59.434 1.000 26.93 ANISOU 1506 CD2 LEU 215 1998 5409 2827 -1083 909 -542 1507 C ATOM LEU 215 15.002 20.622 62.500 1.000 14.65 ANISOU 1507 C LEU 215 1770 1607 2190 86 - 165- 9 5 ATOM 1508 O LEU 215 13.822 20.662 62.151 1.000 19.45 ANISOU 1508 O LEU 215 1748 2165 3476 -303 - 203116 ATOM 1509 N PRO 216 15.552 21.523 63.314 1.000 15.99 ANISOU 1509 N PRO 216 2390 1970 1715 21 - 175-164 1510 CD ATOM PRO 216 16.955 21.601 63.757 1.000 19.37 ANISOU 1510 CD 2155 PRO 216 2900 2306 -83 -790 - 548 1511 CA ATOM PRO 216 14.760 22.620 63.846 1.000 18.68 ANISOU 1511 CA PRO 216 3104 2017 12 -74 - 420 1976 1512 CB ATOM PRO 216 15.649 23.227 64.949 1.000 18.63 ANISOU 1512 CB PRO 1517 216 3592 1971 -120 -4219ATOM 1513 CG PRO 216 17.030 22.847 64.581 1.000 22.35 ANISOU 1513 CG 216 3401 PRO 2426  $-419 \quad -427 \quad -783$ 2666 1514 C ATOM PRO 62.819 216 14.461 23.700 1.000 18.50 ANISOU 1514 C PRO 216 2921 2083 2026 58 - 465 - 473 1515 O ATOM PRO 216 15.024 61.731 23.854 1.000 19.82 ANISOU 1515 O PRO 216 2752 -32 2453 2325 -375 1 9 ATOM 1516 N TYR 217 13.487 24.536 63.194 1.000 20.05 ANISOU 1516 N TYR 217 3213 1981 90 - 482 - 7182422 1517 CA ATOM 217 13.178 TYR 25.662 62.308 1.000 22.97 ANISOU 1517 CA 217 2849 TYR 2652 3227 211 -1467 - 3131518 C ATOM 26.647 TYR 217 14.347 62.283 1.000 23.92 ANISOU 1518 C TYR 217 4139 2819 2131 -337 -1776 -1651519 0. ATOM TYR 217 15.149 26.726 63.213 1.000 30.46 ANISOU 1519 O TYR 217 4321 3440 3812 -1118 -2477 728 1520 CB ATOM TYR 217 11.891 26.314 62.768 1.000 32.68 ANISOU 1520 CB 3294 TYR 217 3958 5164 1148 -874 - 783 1521 CG ATOM TYR 217 12.064 27.462 63.718 1.000 44.77 ANISOU 1521 CG 217 6829 TYR 4326 5854 895 38 - 18701522 CD1 TYR ATOM 217 11.853 28.763 1.000 54.26 63.285 ANISOU 1522 CD1 TYR 217 10311 3688 -323 132 -1945 6615 1523 CD2 TYR ATOM 65.043 1.000 57.77 217 12.428 27.243 ANISOU 1523 CD2 TYR 217 10635 5155 6158 -1027 -1446 -1931 1524 CE1 TYR ATOM 217 12.011 29.816 64.174 1.000 60.33 ANISOU 1524 CE1 TYR 217 11807 4345 -1101 -132 -2259 6772 1525 CE2 TYR 217 12.585 ATOM 28.296 65.926 1.000 64.51 ANISOU 1525 CE2 TYR 217 12481 6832 5199 -1936 -1520 -2074

- 140 -ATOM 1526 CZ 217 12.378 TYR 29.586 65.481 1.000 64.11 ANISOU 1526 CZ TYR 5183 -1460 -817 -2160 217 12047 7129 1527 OH ATOM 66.358 1.000 63.69 TYR 217 12.536 30.639 ANISOU 1527 OH TYR 217 11840 5206 7153 -1832 -1191 -2064 1528 N MOTA 218 14.418 27.374 61.188 1.000 24.08 ARG ANISOU 1528 N ARG 218 4482 1611 3055 507 -1471 - 145218 15.335 ATOM 1529 CA ARG 28.465 60.948 1.000 30.71 ANISOU 1529 CA 218 5932 ARG 2490 3245 -504 -1565 382 ATOM 1530 CB ARG 28.135 59.840 218 16.326 1.000 35.08 ANISOU 1530 CB ARG 218 5969 2797 4562 -1397 -779 - 348 1531 CG 218 17.401 ATOM 27.114 60.073 1.000 35.77 ARG ANISOU 1531 CG ARG 218 6009 3087 4497 -1107 -733 - 773 1532 CD ARG ATOM 218 18.658 60.626 1.000 34.46 27.775 ANISOU 1532 CD 218 5680 ARG 3264 4152 -1242 -244 - 619 1533 NE ATOM ARG 218 19.223 28.746 59.709 1.000 29.51 ANISOU 1533 NE 218 4707 ARG 2579 3926 · 78 81 - 629 1534 CZ ATOM ARG 218 20.218 28.620 58.830 1.000 33.18 ANISOU 1534 CZ ARG 218 5269 3166 4170 60 452 - 1075 1535 NH1 ARG ATOM 218 20.839 27.452 58.709 1.000 27.44 ANISOU 1535 NH1 ARG 218 4202 2881 3341 -503 -373 -1585 1536 NH2 ARG ATOM 218 20.583 29.675 58.077 1.000 22.96 ANISOU 1536 NH2 ARG 218 2327 3579 2817 233 -1117 - 8721537 C 218 14.513 ATOM ARG 29.655 60.464 1.000 31.05 ANISOU 1537 C 218 7353 ARG 1949 2496 -448 -1823 1 9 7 1538 0 ATOM 218 14.114 ARG 29.533 59.295 1.000 40.40 ANISOU 1538 O ARG 218 9873 3235 2241 531 -3168 - 6271539 N ATOM PRO 219 14.246 30.747 61.157 1.000 30.01 ANISOU 1539 N 219 6290 PRO 2559 2555 -499 - 1839 - 284219 14.597 ATOM 1540 CD PRO 31.043 62.543 1.000 36.79 ANISOU 1540 CD PRO 219 8147 2878 2954 -1848 -2548 - 374 ATOM 1541 CA 31.841 60.549 PRO 219 13.464 1.000 26.34 ANISOU 1541 CA PRO 219 4421 3025 2564 -573 -988 - 340 1542 CB ATOM PRO 219 13.523 32.993 61.563 1.000 32.44 ANISOU 1542 CB 219 5361 PRO 2891 4073 -691 -417 - 989 1543 CG ATOM PRO 219 13.947 32.372 62.825 1.000 38.75 ANISOU 1543 CG 219 7916 PRO 3462 3344 -1981 -958 -1235 1544 C ATOM PRO 219 14.005 32.329 59.220 1.000 23.64 ANISOU 1544 C PRO 219 3472 2066 3443 -161 -1028 1 0 9 1545 0 ATOM PRO 219 13.300 32.950 58.412 1.000 30.61 ANISOU 1545 O PRO 219 4358 2934 .4339 -347 -1712 8 7 6 ATOM 1546 N 220 15.269 32.087 58.906 1.000 25.98 ASP ANISOU 1546 N ASP 220 3611 1756 4506 -389 -644 -815 1547 CA ASP 220 15.847 32.660 57.705 1.000 27.96 ATOM ANISOU 1547 CA 220 3951 ASP 1603 5071 -364 30 -824 220 17.212 ATOM 1548 CB ASP 33.238 58.155 1.000 29.61 ANISOU 1548 CB 220 3549 ASP 3142 4558 -176 -326 1 7 6 MOTA 1549 CG ASP 220 18.091 32.158 58.780 1.000 32.09 ANISOU 1549 CG ASP 220 3706 3527 978 615 4961 625 1550 OD1 ASP 220 17.697 ATOM 31.434 59.719 1.000 26.12 ANISOU 1550 OD1 ASP 220 3013 3522 3390 -158 - 289 - 971551 OD2 ASP ATOM 220 19.241 32.088 58.281 1.000 29.09 ANISOU 1551 OD2 ASP 220 3714 3756 3581 304 677 - 712ATOM 1552 C 220 16.037 ASP 31.726 56.525 1.000 25.26 ANISOU 1552 C 220 2508 ASP 5800 1291 1110 - 822 354 1553 0 ATOM ASP 32.095 55.515 1.000 28.28 220 16.641 ANISOU 1553 O 220 4088 · ASP 1665 4994 -855 298 -434 ATOM 1554 N ALA 30.510 56.631 1.000 21.58 221 15.500 ANISOU 1554 N 221 2748 ALA 1770 3681 -288 178 -651 1555 CA ALA ATOM 29.484 55.658 1.000 19.81 221 15.840 ANISOU 1555 CA ALA 221 2986 1452 3090 -342 -224 - 315 ATOM 1556 CB 221 17.130 28.800 56.109 1.000 19.51 ALA

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- 141 -ANISOU 1556 CB ALA 221 2267 3647 1497 -648 45 - 746 ATOM 1557 C ALA 221 14.718 28.469 55.489 1.000 17.71 ANISOU 1557 C ALA 1912 221 2304 -251 -75 -309 2512 ATOM 1558 O 221 13.866 ALA 28.356 56.380 1.000 20.97 ANISOU 1558 O 221 3596 ALA 2029 -503 406 -284 2344 1559 N ATOM 222 14.728 VAL 27.756 54.378 1.000 14.22 ANISOU 1559 N 222 1560 VAL 1582 2262 -76 -92 -11 1560 CA ATOM VAL 222 13.823 26.617 54.160 1.000 14.89 ANISOU 1560 CA 222 1326 VAL 1608 2723 98 - 216 - 205 1561 CB ATOM VAL 222 13.079 26.779 52.830 1.000 17.28 ANISOU 1561 CB VAL 222 1680 1754 3133 90 -657 -144 1562 CG1 VAL 222 13.995 ATOM 26.685 51.620 1.000 19.17 ANISOU 1562 CG1 VAL 222 1974 2625 2686 -446 -775 1 5 0 1563 CG2 VAL 222 11.996 ATOM 25.747 52.641 1.000 17.36 ANISOU 1563 CG2 VAL 222 2185 1879 -254 -362 - 385 2533 1564 C ATOM 222 14.653 VAL 54.263 1.000 12.66 25.339 ANISOU 1564 C 222 1136 VAL 1564 2112 -50 -225 - 378ATOM 1565 O 222 15.828 VAL 25.320 53.893 1.000 13.12 ANISOU 1565 O 222 1280 VAL 1825 1881 104 -13 - 199ATOM 1566 N 223 14.049 LEU 24.267 54.775 1.000 12.98 ANISOU 1566 N 223 1123 LEU 1538 2270  $-163 \quad -370 \quad -417$ 223 14.681 ATOM 1567 CA LEU 22.952 54.749 1.000 10.70 ANISOU 1567 CA 223 891 1704 LEU 1472 -26 -98 - 71568 CB ATOM LEU 223 14.276 22.130 55.961 1.000 13.02 ANISOU 1568 CB LEU 223 1387 1968 1593 289 -108 -419 ATOM 1569 CG LEU 223 14.739 20.683 56.106 1.000 17.41 ANISOU 1569 CG 223 2434 LEU 2132 2050 -290 -476 5 6 6 1570 CD1 LEU ATOM 223 16.247 20.614 56.204 1.000 17.20 ANISOU 1570 CD1 LEU 223 2576 1518 2441 26 - 989 - 249 1571 CD2 LEU ATOM 20.076 57.282 1.000 33.63 223 13.983 ANISOU 1571 CD2 LEU 223 3981 4721 4077 -341 134 2949 1572 C ATOM LEU 223 14.362 22.211 53.456 1.000 10.02 ANISOU 1572 C LEU 223 1000 1543 1265 58 - 319 8 8 ATOM 1573 0 LEU 223 13.206 22.160 53.088 1.000 12.86 ANISOU 1573 O LEU 223 949 1945 -97 1992 -174 - 372ATOM 1574 N 224 15.406 21.675 52.798 1.000 10.55 VAL ANISOU 1574 N 224 978 1070 VAL 1962 -76 -418 - 382ATOM 1575 CA VAL 20.932 51.553 1.000 11.98 224 15:227 ANISOU 1575 CA 224 1376 VAL 1288 1887  $-249 \quad -278 \quad -372$ ATOM 1576 CB 224 16.095 21.461 50.391 1.000 11.23 VAL ANISOU 1576 CB 224 901 1541 VAL 1824 -279 -622224 15.833 20.690 49.102 1.000 13.16 MOTA 1577 CG1 VAL ANISOU 1577 CG1 VAL 224 1899 1485 1615 -462 -516 8 4 1578 CG2 VAL ATOM 224 15.837 22.941 50.156 1.000 13.86 ANISOU 1578 CG2 VAL 224 1480 1520 2266 -135 -354 - 64 ATOM 1579 C VAL 224 15.539 19.450 51.786 1.000 10.87 ANISOU 1579 C VAL 224 953 1275 1901 -13 342 - 484 1580 O ATOM 224 16.646 19.148 52.201 1.000 12.57 VAL ANISOU 1580 O VAL 1363 224 1283 2132 -175 -154 - 274 1581 N ATOM 225 14.585 PHE 18.553 51.533 1.000 11.86 ANISOU 1581 N PHE 225 1241 1128 2137 -15 -303 - 61 1582 CA ATOM 225 14.811 PHE 17.130 `51.412 1.000 11.38 ANISOU 1582 CA PHE 225 1260 1157 -22 -67 - 561909 ATOM 1583 CB 225 13.707 16.280 52.044 1.000 11.34 PHE ANISOU 1583 CB PHE 225 1117 2015 205 -213 3 3 5 1176 ATOM 1584 CG PHE 225 13.654 16.172 53.544 1.000 11.38 ANISOU 1584 CG PHE 225 964 1369 -251 -333 181 1991 1585 CD1 PHE ATOM 225 14.685 15.653 54.291 1.000 15.28 ANISOU 1585 CD1 PHE 225 1771 1777 2256 -98 -853 2 9 8 1586 CD2 PHE ATOM 225 12.532 16.576 54.254 1.000 17.91 ANISOU 1586 CD2 PHE 225 1904 2748 2153 341 106 0

- 142 -1587 CE1 PHE ATOM 225 14.619 15.535 55.661 1.000 17.46 ANISOU 1587 CE1 PHE 225 2449 1862 2321 -249 - 795 6 6 6 225 12.447 1588 CE2 PHE ATOM 16.474 55.612 1.000 19.35 ANISOU 1588 CE2 PHE 225 2563 2678 2111 121 129 - 11 1589 CZ 225 13.499 ATOM PHE 56.341 15.945 1.000 18.20 ANISOU 1589 CZ PHE 225 2952 1641 2324 -501 -470 3 6 1590 C PHE ATOM 225 14.907 16.774 49.927 1.000 12.03 ANISOU 1590 C PHE 225 1480 1285 1804 130 -201421591 0 ATOM PHE 225 14.019 17.160 49.163 1.000 12.77 PHE ANISOU 1591 O 225 1473 1466 1912 341 -118 3 8 226 15.940 1592 N CYS 16.032 49.521 1.000 9.62 ATOM ANISOU 1592 N CYS 226 954 1403 1296 -204 - 407 2 9226 15.917 15.400 48.197 1.000 10.80 ATOM CYS 1593 CA ANISOU 1593 CA 226 1432 CYS 1204 1468 -258 -310 - 59CYS 1594 CB ATOM 226 17.337 15.029 47.744 1.000 12.02 226 1539 CYS ANISOU 1594 CB 1362 1666 -357 16 -125 1595 SG CYS ATOM 226 18.426 16.490 47.554 1.000 13.74 ANISOU 1595 SG CYS 226 1627 2192 1400 -341 18 1 3 9 1596 C 226 14.998 ATOM CYS 14.178 48.256 1.000 9.86 ANISOU 1596 C CYS 226 1190 1061 1495 -20 -293 - 161597 O ATOM 226 15.015 13.431 49.252 1.000 11.17 CYS ANISOU 1597 O CYS 226 1181 -129 -435 2 7 2 1280 1781 GLY 1598 N 227 14.217 ATOM 13.963 47.205 1.000 10.17 ANISOU 1598 N GLY 227 1428 1010 1427 -258 -271 - 35 1599 CA ATOM GLY 227 13.370 12.806 47.053 1.000 9.73 ANISOU 1599 CA GLY 227 1231  $-178 \quad -74 \quad -37$ 860 1604 1600 C 11.769 46.074 1.000 9.48 ATOM 227 13.908 GLYGLY ANISOU 1600 C 227 1438 717 1445 16 -35 1 6 9 1601 0 MOTA GLY227~14.935 11.961 45.402 1.000 9.86 ANISOU 1601 O 227 1321 GLY1137 1290 -104 -179 7 8 1602 N 10.631 45.971 1.000 9.17 ATOM ALA 228 13.217 ANISOU 1602 N ALA 228 1279 729 1477 109 -135 ATOM 1603 CA ALA 228 13.650 9.529 45.108 1.000 9.41 -74 ANISOU 1603 CA ALA 228 1315 887 1371 9 ATOM 45.256 1.000 10.50 1604 CB ALA 228 12.727 8.296 ANISOU 1604 CB ALA 228 2011 824 1155 -143 124 101 MOTA 1605 C 228 13.712 ALA 43.637 1.000 9.25 9.918 ANISOU 1605 C 228 1343 ALA 666 1507 -108 90 1 3 9 1606 0 ATOM ALA 228 14.493 9.305 42.895 1.000 9.48 ANISOU 1606 O 228 1171 1026 -50 9 0 ALA 1405 -88 ATOM ILE 1607 N 229 12.970 10.907 43.143 1.000 10.30 ANISOU 1607 N ILE 229 1402 1004 1509 18 25 177 MOTA 1608 CA ILE 229 13.074 11.311 41.727 1.000 10.87 ANISOU 1608 CA ILE 229 1197 1446 1487 -2 -159 251 1609 CB ATOM ILE 229 11.802 12.078 41.295 1.000 11.52 ANISOU 1609 CB ILE 229 1257 1473 1647 34 - 57 3 6 2 1610 CG2 ILE ATOM 229 11.997 12.852 39.999 1.000 11.30 ANISOU 1610 CG2 ILE 229 1655 1211 1426 83 - 189 156 1611 CG1 ILE ATOM 229 10.575 11.131 41.237 1.000 14.39 ANISOU 1611 CG1 ILE 229 1031 2034 2402 -40 210 311 ATOM 1612 CD1 ILE 229 10.676 40.138 1.000 19.20 10.093 ANISOU 1612 CD1 ILE 229 2085 1723 3489 -610 93 -138 ATOM 1613 C 12.034 ILE 41.477 1.000 10.38 229 14.389 ANISOU 1613 C ILE 229 1293 1405 1247 -62 -169 3 2 2 ATOM 1614 0 ILE 229 14.952 40.369 1.000 11.66 11.947 ANISOU 1614 O ILE -13 145 3 2 8 229 1805 1257 1368 ATOM 1615 N 230 14.965 ALA 12.692 42.490 1.000 10.66 ANISOU 1615 N 230 1476 ALA 1274 1300 -104 -151 3 5 6 ATOM 1616 CA ALA 13.259 42.338 1.000 11.21 230 16.312 ANISOU 1616 CA ALA 230 1473 975 1813 -57 -308 9 0 ATOM 1617 CB ALA 14.148 43.509 1.000 10.58 230 16.681

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- 143 -ANISOU 1617 CB 230 1350 ALA 1295 1375 62 -106 1618 C ATOM 230 17.336 ALA 12.136 42.132 1.000 11.28 ANISOU 1618 C 230 1640 ALA 1037 1610 1 55 2 4 2 1619 0 230 18.220 ATOM ALA 12.185 41.273 1.000 11.29 ANISOU 1619 O 230 1510 1539 ALA 1240 -189 -40 288 THR MOTA 1620 N 231 17.173 11.097 42.946 1.000 10.55 ANISOU 1620 N THR 231 1328 894 1787 -262 -70 2 1 4 THR 231 18.064 ATOM 1621 CA 9.939 42.819 1.000 11.98 ANISOU 1621 CA 231 1929 THR 1605 1018 0 -164 1622 CB 231 17.717 ATOM THR 43.878 1.000 10.76 8.865 ANISOU 1622 CB 231 1381 THR 1070 1636 -86 -453 2 4 6 1623 OG1 THR 231 17.658 ATOM 45.198 1.000 11.82 9.437 ANISOU 1623 OG1 THR 231 1615 1236 1641 35 -115 1624 CG2 THR 231 18.765 ATOM 7.752 43.880 1.000 12.57 ANISOU 1624 CG2 THR 231 1621 1314 1840 160 -89 351 1625 C MOTA 231 17.958 THR 9.352 41.415 1.000 12.52 ANISOU 1625 C THR 231 1632 1500 -145 42 1 1 1624 ATOM 1626 0 231 18.939 THR 9.050 40.732 1.000 12.15 ANISOU 1626 O 231 1636 THR 1233 86 2 2 4 1747 -171627 N 232 16.717 ATOM LEU 40.959 1.000 11.14 9.154 ANISOU 1627 N 232 1608 LEU 1005 1620 90 - 68 1 4 1 1628 CA 232 16.446 ATOM LEU 8.522 39.675 1.000 12.47 ANISOU 1628 CA 232 1880 LEU 1203 1657 109 -16945ATOM 1629 CB 232 14.950 LEU 39.552 1.000 12.81 8.214 ANISOU 1629 CB LEU 232 1989 1225 1654 -78 -209 1 9 ATOM 1630 CG LEU 232 14.452 7.464 38.314 1.000 14.85 ANISOU 1630 CG LEU 232 2171 1753 1719 -5 -410 - 96 1631 CD1 LEU ATOM 232 15.020 6.055 38.240 1.000 16.78 ANISOU 1631 CD1 LEU 232 - 2693 1749 1932 72 -431 232 12.914 ATOM 1632 CD2 LEU 7.411 38.291 1.000 15.70 ANISOU 1632 CD2 LEU 232 2180 1866 1920 -278 -589 4 9 4 1633 C 232 16.964 ATOM LEU 9.354 38.511 1.000 11.58 ANISOU 1633 C LEU 232 1452 1390 1559 309 -301 1 3 6 1634 0 ATOM LEU 232 17.752 37.686 1.000 13.45 8.837 ANISOU 1634 O 232 1808 LEU 1436 1867 320 -17 3 0 1635 N ATOM VAL 233 16.565 10.617 38.414 1.000 10.95 ANISOU 1635 N 233 1428 VAL 1210 1522 -14-2100VAL 1636 CA ATOM 233 16.948 37.242 1.000 11.70 11.421 233 1703 ANISOU 1636 CA VAL 1345 1397 97 5 1 3 1637 CB ATOM VAL 233 16.156 12.743 37.215 1.000 11.14 ANISOU 1637 CB VAL 233 1672 1272 -26 1287 276 ATOM 1638 CG1 VAL 233 16.661 13.774 38.249 1.000 13.34 ANISOU 1638 CG1 VAL 233 1834 1673 1562 -205 653 -368 1639 CG2 VAL ATOM 233 16.106 13.412 35.827 1.000 14.66 ANISOU 1639 CG2 VAL 233 1992 1873 1704 -4 -45 5 8 6 ATOM 1640 C 233 18.459 VAL 11.586 37.132 1.000 13.41 ANISOU 1640 C VAL 233 1712 1573 1811 91 151 1 2 5 ATOM 1641 0 VAL 233 19.012 11.627 36.021 1.000 13.45 ANISOU 1641 O 233 1844 VAL 1402 46 192 4 3 8 1866 THR ATOM 1642 N 234 19.188 11.665 38.250 1.000 13.13 ANISOU 1642 N THR 234 1457 -139 223 126 1639 1893 ATOM 234 20.613 1643 CA THR 11.930 38.244 1.000 13.00 ANISOU 1643 CA THR 234 1483 1600 1855 -188 428 143 1644 CB ATOM THR 234 21.069 12.726 39.465 1.000 12.46 ANISOU 1644 CB 234 1300 THR 1632 1803 200 251 -32 1645 OG1 THR 234 20.825 ATOM 11.941 40.639 1.000 13.71 ANISOU 1645 OG1 THR 234 1660 1662 1888 192 202 291 1646 CG2 THR 234 20.301 ATOM 39.643 1.000 11.37 14.027 ANISOU 1646 CG2 THR 234 1097 1565 1657 -153 -87 169 ATOM THR 234 21.424 10.643 1647 C 38.178 1.000 14.44 ANISOU 1647 C THR 234 1550 1823 2114 6 -73 - 53

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ATOM
       1648 O
                THR
                                 10.710
                     234 22.659
                                        38.233 1.000 15.81
                THR
                     234 1546
ANISOU 1648 O
                                 2169
                                         2293
                                                61 27 2 1 7
                GLY
                     235 20.767
ATOM
       1649 N
                                 9.477
                                         38.070 1.000 14.76
ANISOU 1649 N
                     235 1776
                GLY
                                 1576
                                         2254
                                                77 81 410
       1650 CA
                     235 21.530
ATOM
                GLY
                                 8.249
                                         37.994 1.000 16.69
ANISOU 1650 CA
                GLY
                     235 2053
                                 1803
                                         2486
                                                      35 1 8 9
                                                304
       1651 C
ATOM
                GLY
                     235 22.243
                                 7.862
                                         39.275 1.000 16.83
                                 2031
                GLY
ANISOU 1651 C
                     235 1854
                                         2512
                                                765
                                                      244 193
       1652 0
                     235 23.305
                GLY
                                         39.194 1.000 19.67
ATOM
                                 7.237
ANISOU 1652 O
                GLY
                     235 2074
                                 2172
                                                1035 383 372
                                         3225
       1653 N
                GLY
                                         40.425 1.000 14.46
ATOM
                     236 21.665
                                 8.227
ANISOU 1653 N
                GLY
                     236 1732
                                 1327
                                         2433
                                                154
                                                      198 7 5
       1654 CA
ATOM
                     236 22.187
                GLY
                                         41.692 1.000 15.73
                                 7.768
ANISOU 1654 CA
                GLY
                     236 2060
                                 1381
                                         2536
                                                41 186 3 1 2
       1655 C
                     236 23.166
                                 8.691
MOTA
                GLY
                                         42.388 1.000 14.76
ANISOU 1655 C
                     236 1931
                GLY
                                 1332
                                         2346
                                                252
                                                      73 2 8 8
                GLY
                     236 23.778
ATOM
       1656 0
                                 8.244
                                         43.373 1.000 18.32
ANISOU 1656 O
                     236 1983
                GLY
                                 2197
                                         2782
                                                106
                                                      -105 8 4 4
                     237 23.318
ATOM
       1657 N
                GLN
                                 9.938
                                         41.953 1.000 13.99
ANISOU 1657 N
                     237 1831
                                                158
                GLN
                                 1349
                                         2137
                                                      165 170
                     237 24.209
ATOM
       1658 CA
                GLN
                                 10.956
                                        42.485 1.000 13.13
ANISOU 1658 CA
                     237 1474
                GLN
                                 1304
                                         2210
                                                367
                                                      -31 276
       1659 CB
                     237 24.629
ATOM
                GLN
                                 11.948
                                        41.383 1.000 13.38
ANISOU 1659 CB
                GLN
                     237 1367
                                         2151
                                 1566
                                                99 72 1 5 9
       1660 CG
ATOM
                GLN
                     237 25.390
                                 11.335
                                        40.219 1.000 14.74
                                 1529
ANISOU 1660 CG
                GLN
                     237 1404
                                         2666
                                                518
                                                      410 333
       1661 CD
ATOM
                     237 25.816
                GLN
                                 12.428
                                        39.257 1.000 17.22
                GLN
ANISOU 1661 CD
                     237 2039
                                 2018
                                         2486
                                                -64
                                                      426 360
ATOM . 1662 OE1 GLN
                                 13.208 39.522 1.000 20.60
                     237 26.754
ANISOU 1662 OE1 GLN
                     237 1566
                                 2334
                                         3928
                                                -10
                                                      -29 965
       1663 NE2 GLN
                     237 25.116
MOTA
                                 12.470 38.127 1.000 17.47
ANISOU 1663 NE2 GLN
                                 2093
                                                      438 408
                     237 2014
                                         2533
                                                208
       1664 C
                     237 23.627
ATOM
                GLN
                                 11.739 43.663 1.000 12.90
ANISOU 1664 C
                GLN
                     237 1474
                                 1324
                                         2104
                                                72 -10 2 5 5
       1665 0
ATOM
                     237 24.332
                GLN
                                 12.549 44.282
                                                1.000 15.90
ANISOU 1665 O
                     237 1739
                                 1888
                GLN
                                         2413
                                                -291 \quad 74 \quad -84
MOTA
       1666 N
                                 11.481 44.013 1.000 12.13
                     238 22.365
                VAL
ANISOU 1666 N
                VAL
                                 962 2276
                     238 1372
                                             212
                                                   -33 2 0 0
       1667 CA VAL
MOTA
                     238 21.664
                                 12.182 45.082 1.000 11.91
                     238 1169
ANISOU 1667 CA
                VAL
                                         1920
                                 1436
                                                -121 -276 -19
                VAL 238 20.622 13.158 44.510 1.000 12.00
ATOM
      1668 CB
ANISOU 1668 CB VAL
                    238 1024
                                 1179
                                         2357
                                                -6199-31
       1669 CG1 VAL 238 19.978 13.999 45.601 1.000 13.07
ATOM
ANISOU 1669 CG1 VAL
                     238 1530
                                         1767
                                                63 -232 - 222
                                 1668
       1670 CG2 VAL
MOTA
                     238 21.207
                                 14.088 43.463 1.000 14.00
ANISOU 1670 CG2 VAL
                     238 1795
                                 1470
                                         2053
                                                -40 -2181
                     238 20.990
       1671 C
ATOM
                VAL
                                 11.156 46.000 1.000 13.62
ANISOU 1671 C
                VAL
                     238 1707
                                 1415
                                         2054
                                                 -103 - 40 - 22
MOTA
       1672 0
                                 10.288 45.492 1.000 12.64
                VAL
                     238 20.252
ANISOU 1672 O
                     238 1702
                VAL
                                 977 2123
                                             60 -318 257
       1673 N
ATOM
                     239 21.247
                                 11.246 47.300 1.000 11.99
                LYS
ANISOU 1673 N
                     239 1075
                LYS
                                 1404
                                         2076
                                                 127
                                                      -10174
       1674 CA LYS
ATOM
                     239 20.568
                                 10.444 48.322 1.000 12.77
ANISOU 1674 CA
               LYS
                     239 1224
                                 1541
                                         2088
                                                 -12 -124 8 6
MOTA
       1675 CB
                     239 21.382
                LYS
                                 10.463 49.622 1.000 12.23
ANISOU 1675 CB
                     239 1333
               LYS
                                 1155
                                                 183
                                                     -234 - 28
                                         2158
ATOM
       1676 CG
               LYS
                     239 20.953
                                 9.626
                                         50.793 1.000 13.85
ANISOU 1676 CG
                     239 1643
               LYS
                                 1689
                                         1931
                                                 187 -52 - 8 9
       1677 CD
ATOM
               LYS
                     239 21.927
                                 9.579
                                        51.957 1.000 20.13
ANISOU 1677 CD
                LYS
                      239 2893
                                  1795
                                                 10 -1185 5 8 8
                                        2961
       1678 CE
ATOM
                LYS
                      239 21.364 8.745
                                        53.098 1.000 24.73
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ANISOU 1678 CE	LYS 239 4065	2250 3080	-348 -1465 1064
ATOM 1679 NZ	LYS 239 22.019	8.841 54.420	_
ANISOU 1679 NZ	LYS 239 5658	4315 2293	1610 -930 - 304
ATOM 1680 C	LYS 239 19.169	10.949 48.661	
ANISOU 1680 C	LYS 239 1207	1332 1866	-35 -82 6 4
ATOM 1681 O ANISOU 1681 O	LYS 239 18.976 LYS 239 1638	12.191 48.708	1.000 12.32
ATOM 1682 N	LYS 239 1638 ALA 240 18.222	1294 1749	-2 -25 2 3 6
ANISOU 1682 N	ALA 240 1248	10.047 48.863 1266 1534	
ATOM 1683 CA	ALA 240 16.884	10.368 49.354	-52 -185 - 8 8 1.000 10.21
ANISOU 1683 CA	ALA 240 1292	1057 1531	-195 -37 -109
ATOM 1684 CB	ALA 240 15.784	9.782 48.466	1.000 13.46
ANISOU 1684 CB ATOM 1685 C	ALA 240 1195	2378 1543	-232 20 - 403
ATOM 1685 C ANISOU 1685 C	ALA 240 16.784 ALA 240 1308	9.881 50.807	1.000 10.97
ATOM 1686 O	ALA 240 1308 ALA 240 16.595	1249 1611 8.664 51.059	-127 -142 4 9
ANISOU 1686 O	ALA 240 2136	8.664 51.059 1242 1568	1.000 13.02 -243 28 - 7
ATOM 1687 N	PRO 241 16.967	10.783 51.782	1.000 11.13
ANISOU 1687 N	PRO 241 1723	1041 1466	160 -49 138
ATOM 1688 CD	PRO 241 17.172	12.237 51.654	1.000 11.17
ANISOU 1688 CD ATOM 1689 CA	PRO 241 1419 PRO 241 17.043	1204 1618	-180 -128 7 6
ANISOU 1689 CA	PRO 241 17.043 PRO 241 1597	10.340 53.166 1447 1499	1.000 11.96
ATOM 1690 CB	PRO 241 17.712	1447 1499 11.545 53.891	-172 -32 193 1.000 14.25
ANISOU 1690 CB	PRO 241 1875	1837 1701	-531 -383 2 4 2
ATOM 1691 CG	PRO 241 17.286		1.000 13.61
ANISOU 1691 CG ATOM 1692 C	PRO 241 2015	1446 1709	-596 -465 - 22
ANISOU 1692 C	PRO 241 15.708 PRO 241 1417		1.000 12.35
ATOM 1693 O	PRO 241 14.759		-175 -187 4 1 8 1.000 12.28
ANISOU 1693 O	PRO 241 1359	1582 1723	-232 -468 8 1
ATOM 1694 N	ARG 242 15.700		1.000 12.75
ANISOU 1694 N ATOM 1695 CA	ARG 242 1775	1407 1664	-170 76 2 5 0
ANISOU 1695 CA	ARG 242 14.563 ARG 242 1292		1.000 10.76
ATOM 1696 CB	ARG 242 14.614	1417 1380 7.405 56.223	-207 -281 2 1 1 1.000 15.02
ANISOU 1696 CB	ARG 242 2419	1368 1918	-357 117 294
ATOM 1697 CG	ARG 242 14.115		1.000 17.85
ANISOU 1697 CG	ARG 242 3373	1274 2135	9 -560 251
ATOM 1698 CD ANISOU 1698 CD	ARG 242 14.254		
ATOM 1699 NE	ARG 242 3148 ARG 242 15.667	1111 3120 4.552 55.849	506 503 116
ANISOU 1699 NE	ARG 242 3225	4.552 55.849 2107 2538	1.000 20.71 938 638 212
ATOM 1700 CZ	ARG 242 16.107	3.444 56.416	
ANISOU 1700 CZ	ARG 242 3198	2206 3417	307 -544 5 8 9
ATOM 1701 NH1 ANISOU 1701 NH1			
ATOM 1702 NH2		2112 3083	307 387 195
ANISOU 1702 NH2	ARG 242 17.416	3.184 56.438 2332 3921	1.000 25.41 819 -267 4 0 3
ATOM 1703 C	ARG 242 14.477	9.834 56.704	
ANISOU 1703 C	ARG 242 1571	1463 1506	-248 -214 1 0 7
ATOM 1704 O	ARG 242 15.469	10.377 57.213	1.000 13.65
ANISOU 1704 O ATOM 1705 N	ARG 242 1708 HIS 243 13.252	1439 2040	-322 -401 - 38
ANISOU 1705 N	HIS 243 15.252 HIS 243 1657	10.085 57.118 1410 1342	1.000 11.60 -311 -206 5
ATOM 1706 CA	HIS 243 12.942		-311 -206 5 1.000 11.49
ANISOU 1706 CA	HIS 243 1855		06 -183 140
ATOM 1707 CB ANISOU 1707 CB	HIS 243 12.968	12.462 57.546	1.000 11.22
ATOM 1708 CG	HIS 243 1432 HIS 243 12.133	1379 1453	-231 -221 3 9
ANISOU 1708 CG	HIS 243 12.133 HIS 243 1937	12.694 56.341 1171 1378	
		T710	<del>-</del> 31 -268 7 9

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ATOM	1709	CD2	HIS	243	10.885	13.236	56.181	1.000 11.15
ANISOU	1709	CD2	HIS	243	1990	1106	1142	35 - 344 141
ATOM	1710	ND1	HIS	243	12.538	12.345	55.086	1.000 12.29
ANISOU	1710	ND1	HIS	243	1670	1606	1395	-394 -91 8
ATOM	1711		HIS	243	11.599	12.653	54.209	1.000 12.59
ANISOU	1711	CE1	HIS	243	1686	1740	1357	-522 -202 - 253
ATOM	1712	NE2	HIS	243		13.204	54.841	1.000 10.77
ANISOU	1712		HIS	243	1612	1307	1172	-616 -268 - 36
ATOM	1713		HIS		11.605	10.737	58.812	1.000 12.49
ANISOU	1713		HIS		1869	1570	1308	-321 -53 7 3
ATOM	1714	_	HIS		10.807	9.949	58.271	1.000 12.26
ANISOU ATOM	1714 1715		HIS HIS		1756 11.352	1404	1497 59.983	-188 -115 4 7 1.000 12.16
ANISOU	1715		HIS		1464	11.319 1715	1442	-230 -112 - 3 2
ATOM	1716		HIS	244			60.758	1.000 12.02
ANISOU	1716	CA	HIS		1606	1809	1152	-599 -167 - 24
ATOM	1717	CB	HIS	244	10.255		61.615	1.000 12.51
ANISOU	1717	CB	HIS		1655	1763	1334	-19 101 - 47
ATOM	1718	CG	HIS	244	11.270	9.810	62.698	1.000 15.04
ANISOU	1718	CG	HIS	244	2025	1723	1965	-178 -433 1 5 4
ATOM	1719	CD2	HIS	244	11.276	10.380	63.923	1.000 18.19
ANISOU	1719	CD2	HIS	244	2946	2339	1627	36 - 732 2 9 7
MOTA	1720			244	12.504	9.203	62.662	1.000 19.30
ANISOU					2303	2232	2800	229 -708 2 6 6
ATOM	1721		HIS		13.226	9.387	63.731	1.000 22.48
ANISOU					2649	2734	3159	11 -1206 6 5 0
ATOM	1722			244		10.120	64.531	1.000 22.33
ANISOU				~	3088	2895	2500	-272 -1236 3 8 4 1.000 13.47
ATOM ANISOU	1723 1723		HIS HIS		9.780 1897	1673	61.613 1549	-362 254 6 7
ANISOU	1724		HIS		10.603		61.798	1.000 13.48
ANISOU			HIS		1800	1726	1595	-283 139 -161
ATOM	1725		VAL		8.551		62.130	1.000 15.26
ANISOU			VAL		1852	1964	1983	-417 232 - 55
ATOM	1726		VAL		8.090	13.352		1.000 17.31
ANISOU	1726		VAL		2108	2442	2026	-125 476 -161
ATOM	1727	CB	VAL	245	6.939	14.169	62.360	1.000 17.33
ANISOU	1727	CB	VAL		2094	2473	2019	-80  340  -477
ATOM	1728				6.551			1.000 25.25
ANISOU				245		2966	4410	-137 1939 -1248
ATOM			VAL		7.252	14.713		
ANISOU					3070	2538	2556	-180 313 271
ATOM	1730		VAL		7.682	12.768		1.000 18.29 -443 508 - 71
ANISOU	1731		VAL		2123	2689	2137 64.429	-443 508 - 71 1.000 18.62
ATOM ANISOU		Ī	VAL VAL		6.765 5 1810	11.945 2174	3089	-15 451 2 5 4
ATOM	1732		ALA		8.385	13.202		1.000 21.54
ANISOU			ALA		5 2813	3045		-591 -407 9 0 7
ATOM								1.000 25.10
ANISOU							2379	
ATOM			ALA		5 9.424	12.723	67.537	1.000 29.82
ANISOU			ALA			3408	2540	402 -889 1 3 2 5
MOTA	1735	5 C	ALA		5 7.080	13.545	67.412	1.000 31.20
ANISOU						4143	2632	314 280 4 28
ATOM			ALA		6 6.876	14.714	67.052	1.000 32.39
ANISOU					6 4706	3748	3853	567 1247 - 66
ATOM			ALA		7 6.429	12.973	68.413	1.000 37.30
ANISO			ALA					92 640 8 3 5
ATOM					•			1.000 40 . 42
ANISO		B CA					3878	
MOTA	1/3	9 C	ALA	24	/ 6.289	14.132	2 /0.5/8	3 1.000 42.17

						1-41 -			
ANISOU	1739	C	ALA	247	6495	5891	2626	000 1700 0 4 1	
							3636	-823 1720 3 4 1	
ATOM	1740		ALA	24/	7.048	13.338	71.136	1.000 41.63	
ANISOU	1740	0	ALA	247	5811	6371	3637	-1631 804 425	
ATOM	1741	CB	ALA		4.280				
_						13.067	69.525	1.000 47.17	
ANISOU	1741	CB	ALA	247	5186	9059	3676	-520 523 2683	
ATOM	1742	N	SER	257	1.781	21.848	70.382		
								1.000 31.02	
ANISOU	1742		SER	25/	4109	5558	2119	137 -235 -810	j
$\mathtt{ATOM}$	1743	CA	SER	257	1.214	21.932	69.052	1.000 27.01	
ANISOU	1743	CA	SER		2792				
						5165	2304	109 - 143 - 707	
ATOM	1744	CB	SER	257	0.039	22.914	68.992	1.000 28.16	
ANISOU	1744	CB	SER	257	2655	4473	3572	-238 -90 -107	-
ATOM	1745								1
			SER		0.491	24.251	69.074	1.000 51.32	
ANISOU	1745	OG	SER	257	8516	4131	6853	-616 -2734 -80	17
ATOM	1746	C	SER	257	2.259	22.389	68.034	1.000 26.19	•
ANISOU	1746								
			SER		2537	5064	2 3 5.0	-132 -413 -527	
ATOM	1747	0	SER	257	3.286	22.988	68.352	1.000 31.47	
ANISOU	1747	0	SER	257	2740	5886	3330	-435 -689 -639	ı
ATOM	1748								
			ARG		2.022	22.123	66.763	1.000 26.04	
ANISOU	1748	N	ARG	258	3257	4477	2161	-238 -441 - 19	-
ATOM	1749	CA	ARG	258	2.982	22.541	65.747	1.000 25.81	
ANISOU	1749		ARG						
					2606	4735	2466	73 - 338 - 197	
ATOM	1750		ARG	258	2.321	22.609	64.383	1.000 18.26	
ANISOU	1750	C	ARG	258	2374	2541	2021	39 83 - 854	
ATOM	1751	$\cap$	ARG		1.288				
						21.967	64.131	1.000 19.23	
ANISOU	1751		ARG	258	2600	2819	1888	-389 311 $-420$	ŀ
$\mathtt{ATOM}$	1752	CB	ARG	258	4.188	21.592	65.664	1.000 29.78	
ANISOU	1752	CB	ARG	258	3403	5052			
ATOM	1753						2861	695 -552 - 57	
		CG	ARG		4.246	20.784	64.384	1.000 32.64	
ANISOU	1753	CG	ARG	258	4358	4148	3896	146 97 - 561	
ATOM	1754	CD	ARG	258	5.325	19.746	64.499		
ANISOU	1754		ARG						
					3812	4423	3309	-57 341 $-16$	
ATOM	1755		ARG	258	6.433	19.909	63.581	1.000 29.43	
ANISOU	1755	ΝE	ARG	258	3990	4604	2588	-22 70 5 4 2	
ATOM	1756		ARG		6.453	19.389			
ANISOU	_						62.359	1.000 25.02	
			ARG	258	2540	3893	3074	304 -243 1 0 4	
ATOM	1757	NHl	ARG	258	5.456	18.677	61.835	1.000 22.88	
ANISOU	1757		ARG		2105	2607	3982		
ATOM	1758							359 315 289	
					7.523	19.593	61.617	1.000 22.03	
ANISOU	1758	NH2	ARG	258	2477	2775	3120	-430 -287 -964	,
ATOM	1759	N	THR	259	2.927	23.415	63.527	1.000 20.17	
ANISOU	1759		THR						
					2010	3640	2013	<b>-743</b> 91 <b>-1001</b>	
ATOM	1760		THR	259	2.485	23.505	62.138	1.000 18.33	
ANISOU	1760	CA	THR	259	1801	3043	2121	-533 43 - 685	
ATOM	1761	CB	THR	259	1.821				
ANISOU						24.821	61.713		
	1761		THR		2082	3169	3576	-384 -164 - 580	)
ATOM	1762	OG1	THR	259	2.839	25.830	61.681	1.000 34.27	
ANISOU	1762	0G1	THR		2181	2562	8277		ł
ATOM	1763								i.
			_		0.738	25.198	62.704	1.000 25.49	
ANISOU	1763	CG2	THR	259	4466	2233	2987	325 396 - 948	}
ATOM	1764	C	THR	259	3.702	23.352	61.222	1.000 18.44	
ANISOU	1764	C	THR						
		_			2035	2822	2150	<b>-753 274 -583</b>	,
ATOM	1765		THR	259	4.835	23.698	61.603	1.000 24.74	
ANISOU	1765	0	THR	259	1961	5370	2069	-964 231 -714	j <del>t</del>
ATOM	1766		SER		3.420				•
							60.026		
			SER		1971	2352	1864	-224 2 - 75	
ATOM	1767		SER	260	4.447	22.832	58.989	1.000 17.43	~
ANISOU	1767	CA	SER		1783	2961	1879	321 -95 - 72	
ATOM	1768		SER						
					5.224	21.514	58.956	1.000 20.17	
			SER	260	2306	3257	2100	762 -127 3 8 8	
ATOM	1769		SER	260	4.416	20.392	58.698	1.000 27.09	
ANISOU	1769	OG	SER		3651	2803	3839		
				_ 0 0	J U J 1	2003	2017	426 217 554	

- 148 -ATOM 1770 C SER 260 3.832 23.062 57.614 1.000 14.52 ANISOU 1770 C SER 2165 260 1463 1889 83 -100 SER 260 2.686 ATOM 1771 0 22.681 57.402 1.000 15.92 ANISOU 1771 O SER 260 1513 2489 2049 -93 -1 2 5 7 ATOM 1772 N 261 4.617 SER 23.660 56.742 1.000 13.45 ANISOU 1772 N 261 1489 SER 1832 1788 -190 -120 - 500 1773 CA ATOM SER 261 4.294 23.864 55.334 1.000 13.52 ANISOU 1773 CA SER 261 1599 1726 1812 -204 30 - 315 22.943 1774 C ATOM SER 261 5.209 54.545 1.000 12.45 ANISOU 1774 C SER 261 1332 1887 1513 -42 -240 - 1611775 O ATOM 23.072 54.662 1.000 15.07 SER 261 6.438 ANISOU 1775 O SER 261 1344 1885 2497 -68 -331 - 3431776 CB 261 4.446 SER 25.330 54.943 1.000 17.76 ATOM ANISOU 1776 CB SER 261 2718 2404 1625 **-399 -485 - 318** 1777 OG SER 25.554 53.570 1.000 27.54 ATOM 261 4.428 ANISOU 1777 OG SER 261 4342 3308 2814 -719 -821 9 5 5 1778 N 22.045 53.782 1.000 10.90 MOTA VAL 262 4.623 ANISOU 1778 N 262 1215 VAL 1630 1299 41 -135 1 9 1779 CA ATOM VAL 262 5.393 21.031 53.026 1.000 11.61 ANISOU 1779 CA 1634 VAL 262 1334 1442 156 -103 1 7 1780 CB 262 5.026 19.639 53.558 1.000 11.87 ATOM VAL ANISOU 1780 CB VAL 1614 262 1262 1636 9 - 187 - 741781 CG1 VAL ATOM 262 5.778 18.577 52.779 1.000 13.12 ANISOU 1781 CG1 VAL 262 1462 1997 1527 -2 185 5 1 1782 CG2 VAL ATOM 262 5.262 19.564 55.062 1.000 17.08 ANISOU 1782 CG2 VAL 262 3390 1494 1604 -374 - 245391783 C ATOM VAL 21.149 51.543 1.000 11.18 262 5.096 ANISOU 1783 C VAL 262 1026 1790 1431 1 -111 -138 20.969 51.127 1.000 12.76 ATOM 1784 0 VAL 262 3.939 262 1064 ANISOU 1784 O VAL -251 -84 -2712137 1648 1785 N 21.438 50.714 1.000 9.50 ATOM PHE 263 6.090 ANISOU 1785 N PHE 263 995 1297 1316 -6 -210 -18121.637 49.288 1.000 9.61 ATOM 1786 CA 263 5.933 PHE ANISOU 1786 CA 263 1310 PHE1017 1324 -6 - 284 - 421787 CB ATOM 263 6.486 PHE 23.002 48.848 1.000 10.94 ANISOU 1787 CB PHE 263 1282 1055 1821 -50 1788 CG ATOM PHE 23.399 47.418 1.000 10.35 263 6.150 ANISOU 1788 CG 263 779 1231 -58 PHE 1921 32 3 4 0 1789 CD1 PHE 263 6.858 22.915 46.326 1.000 9.98 ATOM ANISOU 1789 CD1 PHE 263 766 1183 1841 -26 -101 ATOM 1790 CD2 PHE 263 5.106 24.277 47.148 1.000 11.95 ANISOU 1790 CD2 PHE 263 1229 1261 2052 245 -29 261 1791 CE1 PHE 263 6.530 23.229 45.019 1.000 12.49 ATOM ANISOU 1791 CE1 PHE 263 1718 31 - 370 1 3 6 1857 1173 1792 CE2 PHE 263 4.769 24.601 45.836 1.000 13.12 ATOM ANISOU 1792 CE2 PHE 263 1451 1382 2151 43 -292 353 1793 CZ PHE MOTA 263 5.491 24.112 44.762 1.000 12.42 ANISOU 1793 CZ PHE 263 1318 1453 1948 -138 -187 6 4 9 1794 C ATOM PHE 20.505 48.530 1.000 8.91 263 6.636 ANISOU 1794 C PHE 263 1076 1085 1223 -39 -142 2 4 1795 0 MOTA PHE 263 7.868 20.406 48.538 1.000 10.98 ANISOU 1795 O -120 -224 - 145 . PHE 263 1098 1233 .1842 1796 N MOTA PHE 264 5.856 19.691 47.812 1.000 9.19 ANISOU 1796 N PHE 264 1089 -86 -105 - 8 2 1136 1266 1797 CA PHE ATOM 18.602 46.991 1.000 9.64 264 6.386 ANISOU 1797 CA -56 -60 -126 PHE 264 1009 1238 1417 1798 CB ATOM PHE 264 5.483 17.358 47.005 1.000 9.92

ANISOU 1799 CG PHE 264 1241 1647 1374 -121 38 7 7

1201 1359

16.673 48.336 1.000 11.22

16.236 49.139 1.000 15.38

**-78 17** 9

264 1209

1799 CG PHE 264 5.265

1800 CD1 PHE 264 6.292

ANISOU 1798 CB PHE

ATOM

ATOM

£ ...

- 149 -ANISOU 1800 CD1 PHE 264 1467 2641 1734 -225 -8 8 7 3 1801 CD2 PHE 264 3.988 ATOM 16.433 48.808 1.000 16.96 ANISOU 1801 CD2 PHE 264 1425 3252 -610 -79 958 1769 1802 CE1 PHE 264 6.090 ATOM 15.596 50.336 1.000 14.52 ANISOU 1802 CE1 PHE 264 1745 2417 1354 162 334 452 1803 CE2 PHE ATOM 264 3.755 50.019 1.000 18.04 15.796 ANISOU 1803 CE2 PHE 264 1747 3405 -590 -109 1008 1704 264 4.817 ATOM 1804 CZ PHE 15.354 50.779 1.000 12.52 ANISOU 1804 CZ PHE 264 1772 1536 1449 -57 227 334 1805 C 264 6.535 ATOM PHE 19.038 45.533 1.000 8.98 ANISOU 1805 C 264 1103 PHE 919 1392 143 81 - 9 2 1806 O 264 5.497 ATOM PHE 19.368 44.930 1.000 9.79 ANISOU 1806 O 264 991 1190 PHE 28 105 1540 ATOM 1807 N LEU 265 7.758 44.999 1.000 8 . 4 3 19.031 265 992 884 1325 ANISOU 1807 N LEU 173 -180 158 1808 CA MOTA LEU 265 7.984 43.566 1.000 8.66 19.224 ANISOU 1808 CA 265 883 1066 LEU 1339 63 -33 - 7 6 1809 CB 265 9.309 ATOM LEU 19.964 43.328 1.000 10.10 ANISOU 1809 CB LEU 265 1179 1188 1469 -225 -220 2 4 8 ATOM 1810 CG LEU 265 9.570 20.351 41.871 1.000 9.37 ANISOU 1810 CG LEU 265 1072 1009 1478 242 25 1 2 9 1811 CD1 LEU ATOM 265 8.725 21.522 41.408 1.000 10.80 ANISOU 1811 CD1 LEU 265 1291 1004 181 1811 -114 2 9 6 1812 CD2 LEU ATOM 265 11.048 41.678 1.000 10.87 20.684 ANISOU 1812 CD2 LEU 265 1129 1483 1519 134 43 1 4 6 ATOM 1813 C LEU 265 7.933 42.875 1.000 10.21 17.849 ANISOU 1813 C 265 932 1188 LEU -6 -38 1760 ATOM 1814 0 LEU 265 8.858 17.043 43.042 1.000 10.45 ANISOU 1814 O LEU 969 1612 265<sup>2</sup> 1388 84 -217 1 0 7 ATOM 1815 N ARG 266 6.853 17.530 42.135 1.000 10.00 ANISOU 1815 N ARG 266 1325 1069 1404 -120 -22215ATOM 1816 CA ARG 266 6.572 16.198 41.628 1.000 10.50 ANISOU 1816 CA 266 1219 ARG 1217 1554 -294 110 -2101817 CB ATOM ARG 266 5.208 42.124 1.000 10.56 15.675 ANISOU 1817 CB ARG 266 978 1460 1574 -168 -103 -105 1818 CG ATOM 266 4.965 ARG 15.894 43.609 1.000 11.24 ANISOU 1818 CG 266 1337 ARG 1373 1563 119 206 -40 1819 CD ATOM 266 3.668 ARG 44.146 1.000 11.17 15.318 ANISOU 1819 CD ARG 266 1113 1567 1564 -17-49 - 11ATOM 1820 NE ARG 266 2.508 15.879 43.447 1.000 9 . 4 3 ANISOU 1820 NE ARG 266 1341 1157 1086 24 -100 ATOM 1821 CZ ARG 266 1.236 15.509 43.657 1.000 9 . 8 3 ANISOU 1821 CZ ARG 266 1245 1194 1294 132 -159 - 1 1822 NH1 ARG ATOM 266 0.961 44.572 1.000 11.20 14.567 ANISOU 1822 NH1 ARG 266 1208 1240 1806 -144 -454 2 7 2 1823 NH2 ARG ATOM 266 0.225 16.048 42,975 1,000 11,08 ANISOU 1823 NH2 ARG 266 1460 1265 1484 -28373191 ATOM 1824 C ARG 266 6.601 16.190 40.099 1.000 10.28 ANISOU 1824 C ARG 266 1273 1089 1545 -200 -5 -1671825 0 ATOM ARG 266 6.027 39.519 1.000 11.05 17.109 ANISOU 1825 O 266 1254 ARG 1153 1793 -132 47 - 64 ATOM 1826 N PRO 267 7.215 39.496 1.000 10.27 15.162 ANISOU 1826 N PRO 267 1194 1239 1468 -33 130 3 2 1827 CD MOTA PRO 267 7.828 13.963 40.109 1.000 12.36 ANISOU 1827 CD PRO 267.1865 1132 1697 -529 - 192-26 ATOM 1828 CA 267 7.304 PRO 15.157 38.036 1.000 10.12 ANISOU 1828 CA 267 1278 PRO 1095 1472 -129 38 - 185 1829 CB ATOM PRO 267 8.250 13.986 37.767 1.000 11.83 ANISOU 1829 CB 267 1489 PRO 1088 1919 -72 90 - 3221830 CG ATOM 267 8.017 PRO 13.053 38.913 1.000 10.72 ANISOU 1830 CG PRO 267 960 1356 1755 95 -257 -187

	- 150 -	
ATOM 1831 C PRO ANISOU 1832 O PRO ANISOU 1832 O PRO ATOM 1833 N ASN ANISOU 1833 N ASN ANISOU 1834 CA ASN ANISOU 1835 CB ASN ANISOU 1835 CB ASN ANISOU 1835 CB ASN ANISOU 1836 CG ASN ATOM 1836 CG ASN ATOM 1837 OD1 ASN ATOM 1837 OD1 ASN ATOM 1838 ND2 ASN ATOM 1838 ND2 ASN ATOM 1838 ND2 ASN ATOM 1838 ND2 ASN ATOM 1839 C ASN ANISOU 1839 C ASN ATOM 1839 C ASN ATOM 1840 O ASN ATOM 1841 N ALA ANISOU 1841 N ALA ANISOU 1841 N ALA ANISOU 1842 CA ALA ANISOU 1842 CA ALA ANISOU 1842 CA ALA ANISOU 1844 C ALA ANISOU 1845 CB ALA ATOM 1844 C ALA ANISOU 1845 C ALA ATOM 1845 C ALA ANISOU 1846 N ASP ANISOU 1846 N ASP ANISOU 1846 N ASP ANISOU 1846 N ASP ANISOU 1847 CA ASP ANISOU 1846 N ASP ANISOU 1847 CA ASP ANISOU 1848 CB ASP ANISOU 1846 N ASP ANISOU 1847 CA ASP ANISOU 1848 CB ASP ANISOU 1847 CA ASP ANISOU 1847 CA ASP ANISOU 1848 CB ASP ANISOU 1849 CG ASP ANISOU 1840 CB ASP	270 1840 1392 270 7.443 11.290 270 1813 2114 271 7.230 11.911	1378       -261       -341       -300         31.113       1.000       11.92         1595       19       -183       -156         29.850       1.000       14.13         1597       84       111       2         29.777       1.000       15.98         1823       418       -418       564         30.762       1.000       21.61         2312       176       -515       163         28.674       1.000       24.64         2145       -62       -169       13.95         31.264       1.000       12.86         1654       -398       -61       3.15         30.292       1.000       14.83         1709       -346       -141       4         32.439       1.000       11.85
ANISOU 1850 OD1 ASP ATOM 1851 OD2 ASP ANISOU 1851 OD2 ASP ATOM 1852 C ASP ANISOU 1853 O ASP ANISOU 1853 O ASP ANISOU 1854 N PHE ANISOU 1854 N PHE ANISOU 1855 CA PHE ANISOU 1855 CA PHE ANISOU 1856 CB PHE ANISOU 1856 CB PHE ANISOU 1857 CG PHE ANISOU 1857 CG PHE ANISOU 1857 CG PHE ANISOU 1858 CD1 PHE ANISOU 1858 CD1 PHE ANISOU 1858 CD1 PHE ANISOU 1859 CD2 PHE	270 4101       1797         270 4.880       14.152         270 3995       3221         270 6.721       11.542         270 1840       1392         270 7.443       11.290         270 1813       2114         271 7.230       11.911         271 1360       1316         271 8.665       11.927         271 1242       1349         271 1467       1444         271 10.385       11.992         271 1411       1640         271 1513       1516         271 10.624       11.155	2312 176 -515 1 6 3 28.674 1.000 24.64 2145 -62 -169 1 3 9 5 31.264 1.000 12.86 1654 -398 -61 3 1 5 30.292 1.000 14.83 1709 -346 -141 4 9 32.439 1.000 11.85 1824 59 -25 7 0
ANISOU 1859 CD2 PHE ATOM 1860 CE1 PHE ANISOU 1860 CE1 PHE ATOM 1861 CE2 PHE	271 12.779 12.178 271 1432 1760	2131 139 84 2 5 5 34.249 1.000 14.26 2225 -39 46 - 4 1 6 36.019 1.000 15.88

ANISOU 1891 CB

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- 151 -ANISOU 1861 CE2 PHE 271 1537 1818 2679 -263 -675 2 6 0 ATOM 1862 CZ PHE 271 13.006 11.288 35.304 1.000 14.15 ANISOU 1862 CZ PHE 271 1166 1736 2475 7 -531 -467 1863 C ATOM PHE 271 9.259 10.550 32.410 1.000 11.27 ANISOU 1863 C PHE 271 1359 1338 75 271 3 4 8 1585 1864 0 ATOM PHE 271 8.785 9.531 32.920 1.000 12.97 ANISOU 1864 O PHE 271 2011 1320 1596 -85 473 279 ATOM 1865 N 272 10.261 THR 10.498 31.541 1.000 11.95 ANISOU 1865 N 272 1018 THR 1503 2020 -214 300 - 115 MOTA 1866 CA THR 272 10.823 9.254 30.992 1.000 12.70 ANISOU 1866 CA THR 272 1615 1557 1652 132 341 146 ATOM 1867 CB THR 272 10.679 9.281 1.000 16.79 29.450 ANISOU 1867 CB 272 1814 THR 2829 1737 -595 157 -406 1868 OG1 THR ATOM 272 9.301 29.090 1.000 18.02 9.471 ANISOU 1868 OG1 THR 272 1912 2921 2013 -497 -73 1869 CG2 THR ATOM 272 11.200 7.976 1.000 17.02 28.856 ANISOU 1869 CG2 THR 272 2144 2857 1467 538 - 194 -475 ATOM 1870 C THR 272 12.272 9.057 1.000 12.02 31.423 ANISOU 1870 C THR 272 1436 1573 1559 92 603 1 3 7 ATOM 1871 0 THR 272 13.055 10.031 1.000 14.17 31.437 ANISOU 1871 O 272 1451 THR 1583 2351 125 602 412 1872 N ATOM 273 12.625 PHE 7.837 31.828 1.000 12.34 ANISOU 1872 N 273 1402 PHE 1585 17 378 158 1703 ATOM 1873 CA PHE 273 13.953 7.492 32.312 1.000 12.20 ANISOU 1873 CA PHE 273 1362 1364 1909 -126 336 147 ATOM 1874 CB 273 13.951 PHE 7.514 33.861 1.000 12.37 ANISOU 1874 CB PHE 273 1362 -102 1447 1890 211 - 8 1875 CG ATOM PHE 273,12.988 6.528 34.491 1.000 11.65 ANISOU 1875 CG PHE 273 1398 1631 -367 42 - 215 1396 1876 CD1 PHE ATOM 273 11.684 6.889 34.773 1.000 14.11 ANISOU 1876 CD1 PHE 273 1531 2214 1614 -336 293 - 62 1877 CD2 PHE ATOM 273 13.409 5.245 34.803 1.000 13.20 ANISOU 1877 CD2 PHE 273 2024 1639 1352 -358 339 - 9 1878 CE1 PHE ATOM 273 10.793 5.993 35.323 1.000 13.25 ANISOU 1878 CE1 PHE 273 1536 2081 1418 -98 447 4 2 1879 CE2 PHE ATOM 273 12.530 4.329 35.327 1.000 13.39 ANISOU 1879 CE2 PHE 273 1529 1905 1654 -224 140 283 1880 CZ ATOM PHE 273 11.227 4.706 35.604 1.000 14.75 ANISOU 1880 CZ PHE 273 1444 2260 1902 -90 -186 2 7 5 ATOM 1881 C 273 14.423 PHE 6.135 31.795 1.000 12.45 ANISOU 1881 C PHE 273 1278 1526 -120 317 - 31 1927 MOTA 1882 0 273 13.645 5.311 PHE 31.291 1.000 11.95 ANISOU 1882 O PHE 273 1590 1580 -137 226 - 13 1370 1883 N ATOM SER 274 15.717 31.952 1.000 12.07 5.854 ANISOU 1883 N SER 274 1270 1640 1677 -29 558 353 ATOM 1884 CA SER 274 16.335 4.586 31.604 1.000 14.39 ANISOU 1884 CA SER 274 1583 1534 2349 43 707 3 8 4 ATOM 1885 CB 274 17.845 SER 4.771 31.438 1.000 14.49 ANISOU 1885 CB SER 274 1578 1727 2202 213 695 329 1886 OG ATOM 274 18.564 SER 31.424 1.000 14.97 3.558 ANISOU 1886 OG SER 274 1763 1848 2078 349 348 - 13ATOM 1887 C 274 16.100 SER 32.666 1.000 13.12 3.505 ANISOU 1887 C SER 274 1670 8 461 1 3 7 1481 1833 MOTA 1888 O 274 16.438 SER 3.700 33.834 1.000 13.50 ANISOU 1888 O SER 274 1493 1518 2116 -65 119 1 5 ATOM 1889 N VAL 275 15.533 2.359 32.271 1.000 11.90 ANISOU 1889 N VAL 275 1476 -110 490 195 1618 1427 ATOM 1890 CA VAL 275 15.283 33.180 1.000 11.41 1.254 ANISOU 1890 CA VAL 275 1708 1424 1204 -8 286 7 6 1891 CB ATOM 275 14.346 VAL 0.198 32.543 1.000 12.74

1300

1809

62 164 - 16

275 1732

VAL

- 152 -1892 CG1 VAL MOTA 275 14.157 -1.0201.000 16.10 33.437 ANISOU 1892 CG1 VAL 275 2352 1962 -614 -663 3 7 0 1803 1893 CG2 VAL ATOM 275 12.961 0.763 32.261 1.000 13.81 ANISOU 1893 CG2 VAL 275 1535 1786 1924 16 363 1 2 6 275 16.577 1894 C ATOM VAL 33.692 0.622 1.000 12.62 ANISOU 1894 C VAL 275 1574 1594 14 375 1 3 6 1628 1895 O ATOM VAL 275 16.729 0.405 34.926 1.000 13.01 275 1667 ANISOU 1895 O VAL 1643 1634 118 180 1896 N PRO ATOM 276 17.569 0.286 32.889 1.000 14.64 ANISOU 1896. N PRO. 454 - 42276 1583 2066 1914 2 1897 CD ATOM PRO 276 17.583 0.285 31.415 1.000 15.84 ANISOU 1897 CD PRO 276 1565 2536 1916 89 755 3 5 PRO MOTA 1898 CA 276 18.827 -0.25033.453 1.000 16.76 ANISOU 1898 CA PRO 276 1667 2403 2296 261 393 -163 1899 CB PRO ATOM 276 19.732 -0.50332.236 1.000 18.27 276 1804 ANISOU 1899 CB 2568 2571 PRO 411 574 - 142276 18.868 -0.385 1.000 18.96 1900 CG PRO 31.029 ATOM ANISOU 1900 CG PRO 276 2147 2293 725 694 - 372763 1901 C PRO 34.420 1.000 16.32 ATOM 276 19.500 0.710 ANISOU 1901 C 6 7 276 1521 115 PRO 2336 237 2342 1902 0 276 20.035 0.277 35.456 1.000 16.78 ATOM PRO ANISOU 1902 O 276 1411 2689 2275 PRO 93 376 253 1903 N 277 19.475 ATOM LEU 34.155 2.019 1.000 16.58 ANISOU 1903 N 277 1835 2412 2052 LEU -15483 1904 CA LEU ATOM 277 20'.142 2.919 35.099 1.000 17.70 ANISOU 1904 CA LEU 277 1990 2226 2511 362 -21 1905 CB 1.000 20.20 MOTA LEU 277 20.298 4.277 34.425 ANISOU 1905 CB LEU 277: 2952 2292 -1 -14 2 7 1 2432 35.186 1906 CG MOTA LEU 277 21.048 5.359 1.000 20.86 277 2213 LEU ANISOU 1906 CG -355 4 8 2 2221 3490 -321.000 34.24 1907 CD1 LEU ATOM 277 22.446 35.531 4.888 ANISOU 1907 CD1 LEU 277 2157 2303 8552 69 - 8422 5 8 1908 CD2 LEU ATOM 277 21.062 6.620 34.334 1.000 31.91 277 4745 ANISOU 1908 CD2 LEU 2460 4918 -572 1150 -474 1909 C LEU 1.000 16.55 MOTA 277 19.411 2.989 36.430 ANISOU 1909 C LEU 277 1975 1885 2430 211 - 243-218 1910 0 LEU 1.000 19.19 ATOM 277 19.997 3.116 37.517 ANISOU 1910 O 50 1 2 2 LEU 277 2179 2636 2476 -617 1.000 15.48 1911 N ATOM ALA 2.905 36.386 278 18.080 ANISOU 1911 N ALA 279 112 1969 -358 278 2008 1904 ATOM 1912 CA ALA 278 17.308 2.896 37.636 1.000 14.51 ANISOU 1912 CA 278 2109 -309 74 1 6 7 ALA 1763 1641 278 15.814 37.347 1.000 15.41 1913 CB ATOM ALA 2.896 ANISOU 1913 CB ALA 66 301 626 278 2017 1773 2064 38.479 1.000 14.55 1914 C MOTA ALA 278 17.710 1.684 ANISOU 1914 C ALÁ 278 1972 1869 1689 -195 -255 7 9 MOTA 1915 0 278 17.894 1.770 39.683 1.000 13.80 ALA ANISOU 1915 O ALA -250 -166 8 9 278 1444 2144 1655 37.842 1.000 13.86 MOTA 1916 N ARG 279 17.841 0.530 -432 -128 1 6 9 ANISOU 1916 N ARG 279 1795 1728 1742 38.560 1.000 15.88 279 18.242 1917 CA ATOM -0.679ARG ANISOU 1917 CA ARG 279 1995 2064 59 355 4 1 1 1973 -1.922 37.648 1.000 16.83 1918 CB ATOM ARG 279 18.204 279 1889 ANISOU 1918 CB 1897 ARG 2609 84 544 2 5 0 37.291 1.000 19.63 ATOM 1919 CG ARG 279 16.790 -2.323233 9 1 ANISOU 1919 CG 279 2123 2196 3139 -63 ARG 279 16.656 ATOM 1920 CD ARG -3.288 36.131 1.000 27.03 -603 -275 -198 ANISOU 1920 CD ARG 279 3924 3198 3150 -4.578 36.364 1.000 27.45 ATOM 1921 NE ARG 279 17.236 -359 751 -789 279 4659 ANISOU 1921 NE 2854 2915 ARG -5.717 36.779 1.000 32.85 ATOM 1922 CZ ARG 279 16.714

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ANISOU 1922 CZ
                ARG
                     279 4486
                                  3045
                                          4948
                                                  -475 448 -222
       1923 NH1 ARG
ATOM
                     279 15.424
                                  -5.874
                                          37.089
                                                 1.000 29.96
ANISOU 1923 NH1 ARG
                     279 4653
                                  2168
                                          4562
                                                  -103
                                                        967 - 678
       1924 NH2 ARG
                     279 17.551
ATOM
                                  -6.750
                                         36.890
                                                 1.000 37.87
ANISOU 1924 NH2 ARG
                     279 4879
                                  2436
                                         7074
                                                 -276 3278 - 824
       1925 C
MOTA
                     279 19.628
                ARG
                                  -0.519
                                          39.150
                                                 1.000 17.48
ANISOU 1925 C
                     279 2118
                ARG
                                  1653
                                          2871
                                                 75 -8 7 0 5
       1926 O
                     279 19.916
ATOM
                ARG
                                  -1.064
                                                 1.000 26.82
                                          40.212
ANISOU 1926 O
                     279 3764
                ARG
                                  3102
                                          3325
                                                 -1987 -1467 1383
ATOM
       1927 N
                GLU
                     280 20.538
                                  0.189
                                          38.505
                                                 1.000 17.73
ANISOU 1927 N
                GLU
                     280 1983
                                  2293
                                          2459
                                                 109
                                                        609 3 7
       1928 CA
ATOM
                GLÜ
                     280 21.899
                                  0.317
                                                 1.000 19.66
                                          39.026
ANISOU 1928 CA
                     280 2049
                GLU
                                  2023
                                          3396
                                                 125
                                                       215 737
       1929 CB
ATOM
                GLU
                     280 22.836
                                  0.886
                                          37.936
                                                 1.000 20.17
ANISOU 1929 CB
                     280 1648
                GLU
                                         3560
                                  2457
                                                 464
                                                       138 1099
       1930 CG
                     280 22.964
ATOM
                GLU
                                  -0.149
                                         36.818
                                                 1.000 31.79
ANISOU 1930 CG
                GLU
                                  4175
                     280 3477
                                          4427
                                                 801
                                                       1187 - 4
       1931 CD
ATOM
                GLU
                     280 23.698
                                  0.341
                                         35.590
                                                 1.000 39.66
ANISOU 1931 CD
                     280 5144
                GLU
                                  5703
                                          4221
                                                 -64
                                                        1339 - 6
       1932 OE1 GLU
ATOM
                     280 24.466
                                  1.327
                                          35.685
                                                 1.000 39.65
ANISOU 1932 OE1 GLU
                     280 3464
                                  5891
                                          5710
                                                 334
                                                        574 1639
       1933 OE2 GLU
ATOM
                     280 23.489
                                         34.519 1.000 41.55
                                  -0.294
ANISOU 1933 OE2 GLU
                     280 5257
                                  6747
                                         3781
                                                 2245
                                                       -184102
       1934 C
ATOM
                     280 21.984
                GLU
                                  1.188
                                          40.266
                                                 1.000 19.68
ANISOU 1934 C
                     280 1488
                GLU
                                  2350
                                         3640
                                                 -566 162 490
ATOM
                     280 23.031
       1935 0
                GLU
                                  1.142
                                          40.958
                                                 1.000 25.69
ANISOU 1935 O
                     280 1871
                                  3766
                GLU
                                          4123
                                                 231
                                                        -245180
       1936 N
ATOM
                     281.20.943
                CYS
                                          40.565
                                  1.980
                                                 1.000 18.57
ANISOU 1936 N
                     281 1560
                CYS
                                  2609
                                          2887
                                                 -406 -211 1 7 6
       1937 CA
ATOM
                CYS
                     281 21.098
                                  2.762
                                          41.806
                                                 1.000 23.83
ANISOU 1937 CA
                CYS
                     281 3222
                                  2647
                                          3184
                                                 -1189 176 -122
       1938 CB
ATOM
                CYS
                     281 21.079
                                  4.264
                                          41.523
                                                 1.000 25.40
ANISOU 1938 CB
                     281 3278
                CYS
                                  2655
                                          3718
                                                  -426
                                                       368 - 46
       1939 SG
ATOM
                     281 19.587
                CYS
                                  4.904
                                          40.763
                                                 1.000 27.05
ANISOU 1939 SG
                CYS
                     281 3069
                                  2914
                                          4295
                                                 -522
                                                        -37 - 794
ATOM
                     281 20.098
       1940 C
                CYS
                                  2.406
                                         42.907
                                                 1.000 16.99
ANISOU 1940 C
                CYS
                     281 1377
                                         3475
                                  1604
                                                 109
                                                        -6 -546
ATOM
       1941 0
                CYS
                     281 19:971
                                  3.173
                                                 1.000 17.04
                                          43.889
ANISOU 1941 O
                     281 2294
                CYS
                                  1277
                                                 -204 -484 - 129
                                          2902
ATOM
       1942 N
                GLY
                     282 19.447
                                  1.245
                                          42.794 1.000 15.23
ANISOU 1942 N
                     282 1617
                GLY
                                  1597
                                          2572
                                               3 -58 - 436
       1943 CA
ATOM
                GLY
                     282 18.731
                                         43.914 1.000 15.61
                                  0.674
ANISOU 1943 CA
                GLY
                     282 1565
                                                 6 -331 -266
                                  1973
                                         2394
ATOM
       1944 C
                GLY
                     282 17.246
                                  0.519
                                          43.727 1.000 13.75
ANISOU 1944 C
                GLY
                     282 1635
                                  1562
                                          2029
                                                 -270 -446 - 78
ATOM
       1945 0
                GLY
                     282 16.585
                                          44.639 1.000 14.99
                                  0.012
ANISOU 1945 O
                GLY
                     282 1751
                                  1630
                                          2313
                                                 207
                                                      -242 4 5 5
ATOM
       1946 N
                PHE
                     283 16.744
                                  1.009
                                          42.582 1.000 12.65
ANISOU 1946 N
                PHE
                     283 1434
                                  1803
                                                 -200 18 - 252
                                          1570
       1947 CA
ATOM
                     283 15.292
                PHE
                                  0.886
                                          42.374 1.000 11.80
ANISOU 1947 CA
                PHE
                     283 1477
                                  1032
                                                  -15
                                          1974
                                                        -26446
MOTA
       1948 CB
                PHE
                     283 14.839
                                          41.295 1.000 14.13
                                  1.890
ANISOU 1948 CB
                PHE
                     283 2262
                                  972 2136
                                              109
                                                    -187 159
       1949 CG
ATOM
                     283 14.906
                PHE
                                  3.351
                                          41.757 1.000 12.63
ANISOU 1949 CG
                PHE
                     283 1711
                                  1033
                                          2055
                                                  47 -86 9
       1950 CD1 PHE
ATOM
                     283 13.851
                                          42.409 1.000 13.45
                                  3.928
ANISOU 1950 CD1 PHE
                     283 1697
                                  1399
                                          2013
                                                  -166 24 - 229
       1951 CD2 PHE
ATOM
                     283 16.037
                                  4.111
                                          41.519 1.000 13.15
ANISOU 1951 CD2 PHE
                     283 1567
                                  1135
                                          2295
                                                  142
                                                        -41 - 99
       1952 CE1 PHE
ATOM
                    283 13.903
                                  5.248
                                          42.839 1.000 15.61
ANISOU 1952 CE1 PHE
                     283 2111
                                  1649
                                          2171
                                                  -202 484 -617
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1953 CE2 PHE
                    283 16.112 5.432
ATOM
                                        41.963 1.000 12.60
ANISOU 1953 CE2 PHE
                    283 1783
                                937 2068
                                            32 -18
                    283 15.040 5.993 42.641 1.000 13.37
ATOM
      1954 CZ
               PHE
ANISOU 1954 CZ
               PHE
                    283 1863
                                865 2352
                                            187
                                                  -149
      1955 C
                                -0.534 41.972 1.000 11.23
ATOM
               PHE
                    283 14.915
ANISOU 1955 C
               PHE
                                            63 -172 6 5
                    283 1527
                                974 1765
      1956 0
                    283 15.471 -1.071 40.990 1.000 13.24
ATOM
               PHE
ANISOU 1956 O
                                1428
               PHE
                    283 1249
                                        2355
                                               175
                                                    -120 - 361
                    284 13.998
      1957 N
ATOM
               ASP
                                       42.712 1.000 12.31
                                -1.130
ANISOU 1957 N
               ASP
                    284 1607
                                1333
                                               -268 -312 8 7
                                        1736
                    284 13.589
      1958 CA
               ASP
ATOM
                                -2.528
                                       42.527 1.000 12.48
ANISOU 1958 CA
               ASP
                    284 1725
                                1202
                                        1814
                                               -148 -543 3 5 0
ATOM
      1959 CB
               ASP
                    284 13.159
                                -3.156
                                       43.876 1.000 12.67
ANISOU 1959 CB
                    284 2014
               ASP
                                1145
                                        1656
                                               -50
                                                    -406 1 3 5
      1960 CG
ATOM
               ASP
                    284 13.261
                                -4.667
                                        43.909 1.000 13.40
                    284 2077
ANISOU 1960 CG
              ASP
                                1171
                                        1843
                                               110
                                                    -419363
      1961 OD1 ASP
                                -5.246 42.974 1.000 14.98
ATOM
                    284 13.861
ANISOU 1961 OD1 ASP
                    284 1956
                                1094
                                        2640
                                               -87
                                                   11 6 0
      1962 OD2 ASP
ATOM
                    284 12.762
                                -5.306 44.883 1.000 15.79
ANISOU 1962 OD2 ASP
                    284 2494
                                1539
                                        1966
                                               -330 -446 4 3 8
      1963 C
                    284 12.478 -2.641 41.510 1.000 10.82
MOTA
               ASP
ANISOU 1963 C
               ASP
                    284 1238
                                        1487
                                               -205 -99 123
                                1387
ATOM
      1964 0
               ASP
                    284 11.373 -3.100 41.777 1.000 12.28
ANISOU 1964 O
               ASP
                    284 1331
                                1175
                                        2159
                                               -209 48 1 9 1
      1965 N
                    285 12.751 -2.154 40.308 1.000 11.32
ATOM
               VAL
ANISOU 1965 N
                    285 1204
                                1671
               VAL
                                        1426
                                               -93
                                                    -48 6 1
                    285 11.748 -2.062 39.260 1.000 11.45
ATOM
      1966 CA
               VAL
ANISOU 1966 CA
                    285, 1468
               VAL
                                        1500
                                               39 - 219 - 15
                                1384
      1967 CB
                    285 12.153
ATOM
               VAL
                                -1.072 38.157 1.000 11.58
ANISOU 1967 CB
                    285 1412
               VAL
                                1523
                                        1465
                                               -388 -428 - 8
      1968 CG1 VAL
ATOM
                    285 12.278
                                0.362
                                        38.679 1.000 15.02
ANISOU 1968 CG1 VAL
                    285 2209
                                1458
                                        2040
                                               -264 - 442 - 32
      1969 CG2 VAL
MOTA
                    285 13.467
                                -1.482
                                        37.495 1.000 15.70
ANISOU 1969 CG2 VAL
                    285 1909
                                1443
                                        2615
                                               -159 309 447
      1970 C
MOTA
               VAL
                     285 11.424
                                -3.431
                                        38.642 1.000 10.83
ANISOU 1970 C
               VAL
                     285 1232
                                               93 -221 108
                                1281
                                        1602
      1971 0
ATOM
                     285 12.267
               VAL
                                -4.301
                                        38.520 1.000 12.13
ANISOU 1971 O
               VAL
                     285 1214
                                1192
                                        2202
                                               -28
                                                     300 162
      1972 N
               SER 286 10.168 -3.523 38.248 1.000 11.09
ATOM
ANISOU 1972 N
                    286 1116
               SER
                                1608
                                        1489
                                               -76
                                                     967
    1973 CA SER 286 9.558 -4.622 37.510 1.000 11.32
MOTA
ANISOU 1973 CA
               SER
                     286 1104
                                1479
                                        1718
                                               -41 -274 2 5 2
      1974 CB
ATOM
               SER 286 8.483
                                -5.292 38.344 1.000 9 . 8 8
ANISOU 1974 CB
               SER
                     286 1328
                                1141
                                        1285
                                               72 -207 7 0
ATOM
      1975 OG
               SER
                    286 7.570
                                -4.361 38.905 1.000 11.34
ANISOU 1975 OG
               SER
                     286 1391
                                        1729
                                               147 -153 7 5
                                1188
ATOM
       1976 C
                SER
                     286 9.019
                                -4.106 36.175 1.000 10.34
ANISOU 1976 C
               SER
                     286 1127
                                1227
                                        1575
                                               28 -87 2 4 5
       1977 0
ATOM
               SER
                     286 7.829
                                -4.112 35.869 1.000 12.62
ANISOU 1977 O
               SER
                     286 1223
                                2219
                                        1353
                                               0 -178 228
ATOM
       1978 N
               LEU
                     287 9.926
                                 -3.622
                                        35.335 1.000 12.45
ANISOU 1978 N
               LEU
                     287 1414
                                1664
                                        1653
                                               -212 3 161
       1979 CA LEU
ATOM
                     287 9.654
                                -2.900 34.099 1.000 12.59
ANISOU 1979 CA
               LEU
                     287 1622
                                 1558
                                               -366 94 184
                                        1605
                     287 10.145 -1.452 34.210 1.000 12.91
ATOM
       1980 CB
               LEU
ANISOU 1980 CB
               LEU
                     287 1716
                                 1591
                                        1597
                                               -373 -95 2 7
       1981 CG LEU
ATOM
                                 -0.590 35.264 1.000 12.96
                     287 9.452
ANISOU 1981 CG LEU
                     287 1182
                                 1848
                                                -407 -51 -170
                                        1895
       1982 CD1 LEU 287 10.229 0.708
ATOM
                                        35.484 1:000 13.34
ANISOU 1982 CD1 LEU
                    287 1644
                                        2318
                                              -38 -124 2 2 3
                                 1108
       1983 CD2 LEU 287 8.006
ATOM
                                 -0.248 34.914 1.000 14.56
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ANISCU 1983 CD2 LEU 287 1716 1548 2267 36 -550 3 1 8 1984 C ATOM LEU 287 10.319 -3.61032.928 1.000 12.63 ANISCU 1984 C LEU 287 1837 1244 -233 248 354 1719 1985 O ATOM 287 11.529 LEU 32.916 1.000 16.68 -3.805 ANISOU 1985 O 287 1779 LEU 1998 2560 -292 390 -149 1986 N ATOM 288 9:531 ASP -4.045 31.950 1.000 13.91 ANISCU 1986 N ASP 288 2080 1455 223 2 2 7 1751 4 1987 CA ATOM 288 10.079 ASP -4.688 30.759 1.000 15.50 ANISOU 1987 CA 288 2029 ASP 2269 1593 -122 605 153 1988 CB ATOM 288 8.979 ASP 30.043 -5.478 1.000 17.00 ANISOU 1988 CB ASP 288 2722 2125 1613 -250 362 1989 CG ATOM ASP 288 9.480 -6.45229.014 1.000 19.30 ANISOU 1989 CG 288 2467 ASP 2980 1885 173 243 1990 OD1 ASP ATOM 288 10.447 -7.18329.292 1.000 25.95 ANISOU 1990 OD1 ASP 288 2812 3190 501 3856 -239 - 783 1991 OD2 ASP ATOM 288 8.911 -6.508 27.907 1.000 31.76 ANISOU 1991 OD2 ASP 288 5375 4430 2260 1266 -849 -1154 1992 C ATOM 288 10.654 ASP 29.811 1.000 17.08 -3.652ANISOU 1992 C ASP 288 2259 2631 1602 -263 248 534 1993 0 ATOM ASP 288 10.197 -2.50229.708 1.000 23.31 ANISOU 1993 O 288 4276 ASP 2268 2313 -244 -13 ATOM 1994 N 289 11.702 GLY -3.966 29.049 1.000 21.26 ANISOU 1994 N GLY 289 2748 1632 3699 -610 752 5 1 1 1995 CA ATOM GLY 289 12.116 -2.880 28.152 1.000 21.65 ANISOU 1995 CA GLY 289 2842 3988 1396 -1163 71 6 2 6 1996 C ATOM GLY 289 13.084 -1.859 28.736 1.000 22.09 ANISOU 1996 C GLY 289 2888 3509 1996 -738 -23 2 4 3 ATOM 1997 0 GLY 289 13.414 -1.836 29.924 1.000 20.34 ANISOU 1997 O GLY 289 3230 2606 1891 -918 124 147 1998 N ATOM 290 13.562 GLU -0.952 27.869 1.000 16.48 ANISOU 1998 N 290 2665 2099 GLU 1496 222 - 445 5 1999 CA MOTA 290 14.716 GLU -0.11728.182 1.000 16.94 -ANISOU 1999 CA 290 2470 GLU 2161 1806 81 411 - 484 2000 CB ATOM GLU 290 15.579 0.012 1.000 20.26 26.912 ANISOU 2000 CB 290 2670 2740 GLU 2287 414 863 2001 CG ATOM 290 16.071 GLU -1.333 26.386 1.000 24.53 ANISOU 2001 CG GLU 290 3251 3153 2916 664 1218 - 612 ATOM 2.002 CD GLU 290 16.812 27.411 -2.1701.000 27.91 ANISOU 2002 CD GLU 290 3019 3161 4424 989 940 - 2512003 OE1 GLU ATOM 290 17.874 -1.74727.917 1.000 35.13 ANISOU 2003 OE1 GLU 290 3913 4458 4975 963 290 16.336 2004 OE2 GLU ATOM -3.280 27.734 1.000 43.76 ANISOU 2004 OE2 GLU 290 6893 6478 3257 -30 -748 5 9 8 2005 C ATOM GLU 290 14.406 1.271 28.716 1.000 14.67 ANISOU 2005 C GLU 290 2512 1756 1308 95 142 1 0 ATOM 2006 O 290 15.260 GLU 29.412 1.000 15.25 1.840 ANISOU 2006 O GLU 290 2074 1969 1750 50 418 - 262 2007 N ATOM 291 13.232 THR 28.437 1.000 15.72 1.814 ANISOU 2007 N THR 291 2173 2393 1406 78 346 - 519 ATOM 2008 CA 291 12.792 THR 3.087 28.991 1.000 15.16 ANISOU 2008 CA 291 2080 THR 1845 1833 -88 631 - 15ATOM 2009 CB THR 291 12.766 27.956 1.000 18.67 4.226 ANISOU 2009 CB 291 2724 THR 2529 1842 -361 769 336 ATOM 2010 OG1 THR 291 11.756 4.009 26.976 1.000 22.93 ANISOU 2010 OG1 THR 291 3313 3135 2265 445 78 1 4 6 2011 CG2 THR MOTA 291 14.096 27.213 1.000 21.82 4.306 ANISOU 2011 CG2 THR 291 3035 3130 2126 357 1450 9 0 2 2012 C ATOM 291 11.402 THR 29.622 1.000 12.86 2.920 ANISOU 2012 C 291 1863 THR 1604 1421 47 305 219 ATOM 2013 O 291 10.625 THR 29.270 1.000 16.13 2.024 ANISOU 2013 O 291 2344 THR 1983 1804 -303 750 -431

- 156 -292 11.037 3.791 MOTA 2014 N ALA 30.542 1.000 12.41 ALA ANISOU 2014 N 292 1495 1363 1859 -2 256 7 7 2015 CA ALA MOTA 292 9.746 3.839 31.202 1.000 11.57 ANISOU 2015 CA ALA 1257 1779 -213 292 1362 153 3 7 2016 CB 2.954 MOTA ALA 292 9.718 32.439 1.000 12.62 ANISOU 2016 CB ALA 292 1768 1245 1784 100 357 4 292 9.385 2017 C MOTA ALA 5.255 31.614 1.000 10.32 ANISOU 2017 C ALA 1335 1270 292 1317 -181 99 5 4 2018 0 MOTA ALA 292 10.266 6.134 31.701 1.000 10.97 ANISOU 2018 O 1138 ALA 292 1389 -146 279 104 1641 2019 N THR 293 8.091 5.445 MOTA 31.882 1.000 12.32 ANISOU 2019 N THR 293 1486 1547 1647 -314 563 -284 293 7.626 2020 CA ATOM THR 6.715 32.421 1.000 12.28 293 1717 ANISOU 2020 CA THR 1460 1489 -168 337 - 2002021 CB THR 293 6.352 ATOM 7.215 31.733 1.000 13.27 ANISOU 2021 CB THR 293 2128 1182 -258 -159 - 284 1730 2022 OG1 THR ATOM 293 5.317 6.237 31.911 1.000 13.85 ANISOU 2022 OG1 THR 293 1831 1217 2216 8 - 131 7 42023 CG2 THR 293 6.474 ATOM 7.303 30.212 1.000 13.72 ANISOU 2023 CG2 THR 293 1791 1683 1738 -252 -56 -405 2024 C 293 7.363 THR ATOM 6.635 33.937 1.000 10.58 ANISOU 2024 C THR 293 1439 1050 1533 12 447 9 2025 0 THR 293 7.211 34.553 ATOM 5.576 1.000 10.29 ANISOU 2025 O THR 293 1049 1102 1758 -56 93 1 1 8 2026 N PHE 7.810 ATOM 34.569 294 7.243 1.000 11.53 ANISOU 2026 N PHE 294 1794 1093 1494 -307 306 - 66 ATOM 2027 CA PHE 294 6.806 7.939 35.950 1.000 10.41 ANISOU 2027 CA 294.1432 1061 1463 -174 125 -162PHE PHE ATOM 2028 CB 294 6.709 36.336 1.000 12.25 9.426 ANISOU 2028 CB PHE 294 1930 1030 1694 -164 292 -64ATOM 2029 CG PHE 294 6.270 9.658 37.770 1.000 12.77 294 1880 ANISOU 2029 CG -103 178 -427PHE 1136 1837 9.462 ATOM 2030 CD1 PHE 294 7.123 38.839 1.000 14.73 ANISOU 2030 CD1 PHE 294 1976 1893 1727 -539 161 -132 2031 CD2 PHE 294 4.989 38.056 1.000 16.59 ATOM 10.068 294 2180 ANISOU 2031 CD2 PHE 1923 2199 386 - 492348 2032 CE1 PHE ATOM 294 6.726 9.673 40.144 1.000 14.36 ANISOU 2032 CE1 PHE **-**505 280 - 118 294 1598 1830 2028 2033 CE2 PHE 294 4.575 ATOM 10.275 39.345 1.000 16.75 ANISOU 2033 CE2 PHE 144 - 602 294 2214 2062 2087 692 ATOM 2034 CZ PHE 294 5.426 10.065 40.413 1.000 15.17 ANISOU 2034 CZ PHE 294 2040 2296 327 1426 2035 C PHE 294 5.484 7.195 36.172 1.000 10.89 ATOM PHE 294 1401 ANISOU 2035 C 1200 1536 -155 78 1 3 7 2036 0 ATOM PHE 294 5.325 6.425 37.125 1.000 10.67 ANISOU 2036 O PHE 1297 294 1396 1360 90 337 1 0 5 ATOM 2037 N 35.299 1.000 10.62 295 4.487 7.355 GLNGLN 295 1399 ANISOU 2037 N 1187 1450 -18 88 - 24 2038 CA GLN 6.612 ATOM 295 3.217 35.393 1.000 11.31 ANISOU 2038 CA GLN -96 120 -321 295 1433 1205 1660 2039 CB 295 2.284 MOTA GLN 7.053 34.254 1.000 11.66 ANISOU 2039 CB GLN 295 1425 -25 63 - 141 1053 1953 2040 CG GLN 295 0.951 34.200 1.000 11.05 ATOM 6.360 ANISOU 2040 CG GLN -93 -118 1 8 295 1573 1011 1614 2041 CD GLN ATOM 295 0.052 6.843 33.087 1.000 11.35 ANISOU 2041 CD GLN 295 1592 1326 1395 173 57 - 13 7.823 2042 OE1 GLN 295 0.349 32.378 1.000 15.06 ATOM ANISOU 2042 OE1 GLN 295 2306 1589 7 3 7 9 182,5 - 110 ATOM. 2043 NE2 GLN 295 -1.053 6.153 32.914 1.000 13.90 ANISOU 2043 NE2 GLN 295 1511 1757 2015 156 -282 2 0 8 2044 C GLN 295 3.412 5.107 ATOM 35.389 1.000 10.12

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- 157 -ANISOU 2044 C GLN 295 1154 1203 1486 21 160 - 191 MOTA 2045 O GLN 295 2.827 4.309 36.128 1.000 11.82 ANISOU 2045 O GLN 295 1264 1542 1686 -107 41 1 3 7 296 4.267 MOTA 2046 N ASP 4.558 34.538 1.000 9.35 ANISOU 2046 N ASP 296 1076 1056 1422 -118 -76 -275 2047 CA 296 4.655 ATOM ASP 1.000 9 . 9 1 3.172 34.416 ANISOU 2047 CA ASP 296 1241 1139 1387 56 60 - 243 2048 CB ATOM ASP 296 5.699 33.347 2.852 1.000 10.26 ANISOU 2048 CB 296 1315 ASP 1156 1429 113 132 - 362049 CG 296 5.343 ASP ATOM 2.981 31.885 1.000 11.42 ANISOU 2049 CG ASP 296 1357 1578 1405 358 121 - 1992050 OD1 ASP 296 4.143 ATOM 31.531 2.904 1.000 13.82 ANISOU 2050 OD1 ASP 296 1511 1744 1997 149 -209 - 622051 OD2 ASP ATOM 296 6.282 3.151 31.047 1.000 13.48 ANISOU 2051 OD2 ASP 296 1802 1758 1564 228 364 2052 C 296 5.175 MOTA ASP 2.682 35.770 1.000 10.31 ANISOU 2052 C 296 1416 ASP 1141 1361 16 91 - 198 ASP 296 4.852 MOTA 2053 0 1.551 36.197 1.000 11.40 ANISOU 2053 O 296 1428 ASP 1452 1453 -288 32 3 5 2054 N ATOM TRP 297 6.004 3.484 36.441 1.000 10.88 ANISOU 2054 N 297 1752 TRP 1144 1238 -161 11 5 5 297 6.646 TRP ATOM 2055 CA 3.104 37.685 1.000 11.26 ANISOU 2055 CA TRP 297 1768 1215 1294 -217 -57 2056 CB ATOM TRP 297 7.899 3.999 37.890 1.000 10.31 ANISOU 2056 CB TRP 1112 297 1387 1417 -87 213 120 2057 CG ATOM TRP 297 8.621 3.651 39.172 1.000 10.98 ANISOU 2057 CG TRP 297 1456 1394 1324 164 -29 - 432058 CD2 TRP ATOM 297 9.082 4.534 40.202 1.000 12.49 ANISOU 2058 CD2 TRP 297 1255 1729 1761  $75 - 298 \cdot - 197$ 2059 CE2 TRP 297 9.692 MOTA 41.201 1.000 16.08 3.755 ANISOU 2059 CE2 TRP 297 1860 2049 2202 -294 -977 4 9 2060 CE3 TRP ATOM 297 9.040 5.910 40.379 1.000 17.41 ANISOU 2060 CE3 TRP 297 2778 1740 2096 -388 - 916 - 2342061 CD1 TRP MOTA 297 8.969 2.400 39.589 1.000 13.58 ANISOU 2061 CD1 TRP 297 1617 1518 2025 0 -664 1 1 4 2062 NE1 TRP ATOM 297 9.614 2.444 40.808 1.000 16.12 ANISOU 2062 NE1 TRP 297 2165 1909 2051 -22 -873 2 2 0 2063 CZ2 TRP ATOM 297 10.243 4.320 1.000 19.85 42.341 ANISOU 2063 CZ2 TRP 297 2756 2383 2404 -951 -1337 267 2064 CZ3 TRP 297 9.586 ATOM 41.515 6.466 1.000 23.40 ANISOU 2064 CZ3 TRP 297 4215 2030 2645 -1001 - 1757 - 77297 10.181 2065 CH2 TRP ATOM 42.486 1.000 21.51 5.670 ANISOU 2065 CH2 TRP 297 3178 2457 2537 -910 -1473 - 51 2066 C ATOM TRP 297 5.700 38.882 1.000 10.39 3.138 ANISOU 2066 C TRP 297 1172 1448 1329 -280 -237 3 9 1 2067 0 ATOM TRP 297 5.574 2.159 39.639 1.000 13.52 ANISOU 2067 O TRP 1830 1557 32 - 91 7 0 3 297 1748 2068 N ATOM 298 5.033 39.079 1.000 12.08 ILE 4.272 ANISOU 2068 N ILE 298 1400 1710 83 4 5 1 1480 -49 ATOM 2069 CA ILE 298 4.223 4.521 40.272 1.000 13.43 ANISOU 2069 CA ILE 298 1301 -199 - 158 - 331317 2484 MOTA 2070 CB ILE 298 4.370 1.000 16.97 5.988 40.689 ANISOU 2070 CB 298 1877 ILE 2908 1661 -1000214 - 630ATOM 2071 CG2 ILE 298 3.538 6.423 1.000 22.01 41.876 ANISOU 2071 CG2 ILE 298 3980 3121 1263 -233 546 -339 2072 CG1 ILE ATOM 298 5.847 6.253 41.037 1.000 27.10 ANISOU 2072 CG1 ILE 5151 298 2588 2557 -2140 -708 9 7 2073 CD1 ILE MOTA 298 6.365 5.522 42.266 1.000 43.13 ANISOU 2073 CD1 ILE 298 5185 8299 2904 -3717 -3055 7 0 8 2074 C ATOM ILE 298 2.772 4.116 40.131 1.000 10.94 ANISOU 2074 C ILE 298 1350 1652 -165 -79 9 6 1156

- 158 -ATOM 2075 0 ILE 298 2.137 3.844 41.155 1.000 12.67 ANISCU 2075 O ILE 298 1689 1634 1493 -102 212 352 299 2.267 4.077 GLY ATOM 2076 N 1.000 10.14 38.897 GLY 299 1412 ANISOU 2076 N 1057 1384 -51 -377 2 0 1 299 0.866 2077 CA GLY ATOM 38.695 1.000 10.72 3.822 299 1335 ANISOU 2077 CA GLY 1084 1655 0 - 229 - 2062078 C 299 0.049 ATOM GLY 5.054 38.369 1.000 12.05 ANISOU 2078 C 299 1422 GLY 1293 1864 105 -29202079 0 GLY ATOM 299 0.585 6.088 37.976 1.000 13.11 ANISOU 2079 O GLY 299 1917 1199 1866 174 80 - 23GLY ATOM 2080 N 300 - 1.2684.931 38.490 1.000 13.92 GLY ANISOU 2080 N 300 1393 1531 2363 182 -410 - 223GLY ATOM 2081 CA 300 - 2.2375.932 38.087 1.000 14.02 ANISOU 2081 CA GLY 300 1524 1471 217 2331 -563 - 336 2082 C GLY ATOM 300 -2.587 7.015 39.074 1.000 11.97 ANISOU 2082 C 2004 GLY 300 940 1603 67 -488 -295 GLY 2083 0 300 -3.322 7.950 ATOM 38.722 1.000 10.90 ANISOU 2083 O GLY 300 1219 1408 1515 -37 -203 - 134301 -2.090 ASN ATOM 2084 N 40.285 1.000 11.64 6.910 ANISOU 2084 N ASN 301 948 1557 -383 -327 165 1917 2085 CA ATOM ASN 301 -2.195 7.915 41.323 1.000 13.39 ANISOU 2085 CA ASN 301 1626 1904 1557 -191 -403 1 8 3 ATOM 2086 CB ASN 301 -3.047 7.301 42.427 1.000 17.60 ANISOU 2086 CB ASN 301 1391 2869 2426 -9 326 2 2 8 ATOM 2087 CG ASN 301 -4.021 8.196 43.108 1.000 19.15 ANISOU 2087 CG 301 2549 ASN 1900 805 2827 59 3 7 7 2088 OD1 ASN 301 -5.072 ATOM 8.606 42.591 1.000 15.47 ANISOU 2088 OD1 ASN 2340 301:1258 2280 -253 339 - 8301 -3.661 2089 ND2 ASN 8.510 ATOM 44.367 1.000 29.28 ANISOU 2089 ND2 ASN 301 3585 4783 2758 1521 -850 - 885 2090 C ATOM ASN 301 -0.862 8.331 41.914 1.000 11.31 ANISOU 2090 C ASN 301 1436 1669 1194 1 1 -168 301 -0.033 ATOM 2091 0 ASN 7.456 42.221 1.000 12.03 ANISOU 2091 O ASN 301 1483 1548 1542 -151 -279 8 2 302 -0.634 ATOM 2092 N TYR 9.628 42.133 1.000 11.53 ANISOU 2092 N 302 1186 TYR 1584 1611 -61 26 1 0 2 2093 CA 302 0.573 MOTA TYR 10.046 42.838 1.000 11.90 ANISOU 2093 CA 302 1260 TYR 1395 1865 5 -212 225 2094 CB 302 0.657 11.589 43.036 1.000 13.14 MOTA TYR 302 1768 ANISOU 2094 CB TYR -273 190 181 1820 1404 ATOM 2095 CG TYR 302 1.082 12.287 41.750 1.000 10.88 ANISOU 2095 CG TYR 302 1395 1347 1393 -321 2 -1532096 CD1 TYR 302 2.421 MOTA 12.439 41.413 1.000 11.29 ANISOU 2096 CD1 TYR 302 1385 1659 -58 98 - 46 1246 2097 CE1 TYR 302 2.859 ATOM 40.248 1.000 10.60 13.075 ANISOU 2097 CE1 TYR 302 1055 1241 1732 -11 52 -1MOTA 2098 CD2 TYR 302 0.161 12.793 40.858 1.000 11.30 ANISOU 2098 CD2 TYR 302 1304 1332 1656 -145 105 - 2.62099 CE2 TYR 302 0.573 ATOM 13.406 39.690 1.000 11.72 ANISOU 2099 CE2 TYR 302 1013 1733 -288 -138 1 6 1 1708 2100 CZ ATOM TYR 13.551 39.375 1.000 10.35 302 1.907 ANISOU 2100 CZ TYR 302 1009 1214 -229 -50 -191709 ATOM 2101 OH TYR 302 2.284 14.153 38.202 1.000 11.82 ANISOU 2101 OH TYR 302 1192 1532 1766 -8 102 1 0 4 2102 C ATOM TYR 302 0.654 9.349 44.196 1.000 12.45 ANISOU 2102 C TYR 302 1517 1450 1765 -181 -202 2 1 72103 O 302 -0.375 ATOM TYR 9.230 44.878 1.000 13.55 ANISOU 2103 O TYR 302 1464 1925 1759 -339 -211 7 MOTA 2104 N VAL 303 1.868 8.967 44.542 1.000 12:06 ANISOU 2104 N VAL 303 1517 1653 -135 -3 3 4 0 1413 2105 CA ATOM VAL 303 2.309 8.430 45.820 1.000 11.88

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- 159 -ANISOU 2105 CA 303 1434 VAL 1609 -368 -197 2 2 3 1471 303 2.755 2106 CB ATOM VAL 6.967 45.736 1.000 14.57 303 1395 ANISOU 2106 CB VAL 1682 2459 -217 -918 3 1 2 2107 CG1 VAL 303 3.131 ATOM 6.462 47.132 1.000 17.33 ANISOU 2107 CG1 VAL 303 2644 1608 2331 -48 -1114 6 1 2108 CG2 VAL 303 1.703 ATOM 6.041 45.122 1.000 14.80 ANISOU 2108 CG2 VAL 303 1876 1676 2069 -592 -639 3 2 2 2109 C ATOM 303 3.467 VAL 9.328 46.303 1.000 13.88 ANISOU 2109 C VAL 303 870 1791 2613 75 -286 - 375 2110 0 ATOM VAL 303 4.526 45.681 1.000 19.70 9.417 ANISOU 2110 O 303 1064 VAL 2307 4114 -61 323 - 999 2111 N · 304 3.271 ATOM ASN 10.046 1.000 13.77 47.393 ANISOU 2111 N ASN 304 1681 1815 -479 -388 1 4 0 1737 ASN ATOM 2112 CA 304 4.205 11.077 47.828 1.000 13.37 ANISOU 2112 CA 304 1626 ASN 1240 2212 -213 -533 2 7 9 ATOM 2113 CB ASN 304 3.460 12.223 48.566 1.000 13.24 ANISOU 2113 CB ASN 304 1206 1454 2370 -243 -344296ATOM 2114 CG ASN 304 2.457 12.922 47.667.1.000 14.16 ANISOU 2114 CG ASN 304 1142 2326 1910 146 -88 230 2115 OD1 ASN ATOM 13.283 304 2.776 1.000 16.65 46.540 ANISOU 2115 OD1 ASN 304 1408 2456 2464 107 185 916 2116 ND2 ASN 304 1.263 ATOM 13.126 48.209 1.000 17.45 ANISOU 2116 ND2 ASN 304 1414 2961 2257 545 181 2117 C ATOM ASN 304 5.325 10.588 1.000 11.18 48.728 ANISOU 2117 C ASN 304 1382 1299 1566 -183 -163 1 1 2 MOTA 2118 0 ASN 304 6.396 11.232 48.699 1.000 12.07 ANISOU 2118 O ASN 304 1325 1382 1879 -167 -66 - 59 ATOM 2119 N ILE 305 5.092 9.541 49.516 1.000 12.56 ANISOU 2119 N ILE 305~1791 1296 1685 -152 -232 2 0 2 2120 CA ATOM 305 6.063 ILE 1.000 14.01 9.011 50.463 ANISOU 2120 CA ILE 305 2314 1393 1614 -55 -479 7 9 2121 CB 305 5.781 ATOM ILE 9.493 51.906 1.000 14.44 ANISOU 2121 CB 305 2223 ILE 1604 1659 -29 -217157ATOM 2122 CG2 ILE 305 5.725 11.017 51.956 1.000 15.31 ANISOU 2122 CG2 ILE 305 1768 1608 2441 43 - 479- 3 1 4 2123 CG1 ILE ATOM 305 4.543 8.853 52.498 1.000 14.83 ANISOU 2123 CG1 ILE 305 1779 1694 27 - 3072163 -153 2124 CD1 ILE ATOM 305 4.163 9.252 1.000 28.68 53.900 ANISOU 2124 CD1 ILE 305 3788 5324 1786 -1491 381 2125 C ATOM 305 6.059 ILE 50.389 7.487 1.000 12.79 ANISOU 2125 C 305 1703 ILE 1355 -260 1800 -586 2 3 1 305 5.111 ATOM 2126 0 ILE 6.864 49.897 1.000 15.63 ANISOU 2126 O 305 1779 ILE 1564 -185 -1008 2 7 7 2597 ATOM 2127 N ARG 306 7.170 6.896 50.829 1.000 13.04 ANISOU 2127 N ARG 1389 306 1618 1946 -368 -598 3 8 3 2128 CA ATOM ARG 306 7.340 5.435 50.868 1.000 11.82 ANISOU 2128 CA 306 1352 ARG -375 -154 4 4 4 1366 1773 2129 CB ARG ATOM 306 8.111 4.965 49.640 1.000 15.28 ANISOU 2129 CB ARG 306 1976 1941 1886 -368 -19 111 ATOM 2130 CG 306 8.203 ARG 3.472 49.395 1.000 17.16 ANISOU 2130 CG 306 2566 ARG 1953 2001 -68 -68 7 6 ATOM 2131 CD 306 8.344 ARG 3.075 47.937 1.000 19.51 ANISOU 2131 CD ARG 306 2921 2361 -397 -396 - 302 2130 2132 NE MOTA ARG 306 7.078 47.212 1.000 20.65 3.198 ANISOU 2132 NE ARG 306 2693 2844 2309 -1056 -310 2 1 4 2133 CZ **MOTA** ARG 306 6.948 3.186 45.893 1.000 17.11 ANISOU 2133 CZ ARG 306 2006 2225 2268 45 - 91 5 9 6 2134 NH1 ARG ATOM 306 8.013 3.065 45.083 1.000 21.58 ANISOU 2134 NH1 ARG 306 2405 2677 3116 -232 381 -669 2135 NH2 ARG ATOM 306 5.734 3.301 45.365 1.000 17.51 ANISOU 2135 NH2 ARG 306 2235 1550 2868 150 -484 - 162

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ATOM	2136	-	ARG	306 8.035	5.027	52.155	1.000 13.45
ANISOU ATOM	2136 2137		ARG	306 2254	1018	1837	-246 -481 9 8
ANISOU	2137	_	ARG ARG	306 9.006 306 1902	5.682 1099	52.556 1615	1.000 12.15 -18 -362 - 80
ATOM		N	ARG	307 7.571	3.968	52.811	1.000 18.19
ANISOU		N	ARG	307 3073	1620	2218	-734 -938 7 9 2
ATOM		CA	ARG	307 8.197	3.380	53.989	1.000 19.20
ANISOU ATOM	2139 2140		ARG ARG	307 3053 307 9.086	1963 2.191	2277 53.611	-675 -1236 6 4 3 1.000 23.08
ANISOU	2140		ARG	307 4018	1905	2847	-270 -1885 3 2 9
ATOM	2141	0	ARG	307 8.636	1.292	52.895	1.000 35.93
ANISOU	2141	0	ARG	307 6003	2403	5244	38 - 3227 - 791
ATOM ANISOU	2142 2142	CB	ARG ARG	307 7.131 307 5557	2.918 3297	54.997 1882	1.000 28.25 -1503 -277 5 0 9
ATOM		CG	ARG	307 6.032	3.921	55.275	1.000 33.39
	2143	CG	ARG	307 4564	4859	3261	-1613 731 2 0 8
ATOM	2144	CD	ARG	307 5.022	3.523	56.317	1.000 40.42
ANISOU ATOM	2144 2145	NE	ARG ARG	307 6335 307 5.605	5701 2.952	3322 57.529	-1900 1263 9 7 1 1.000 50.83
ANISOU	2145		ARG	307 8119	7287	3908	-2786 105 1624
ATOM	2146	CZ	ARG	307 4.894	2.441	58.530	
ANISOU ATOM	2146 2147		ARG	307 7424	8064	4025	-3650 -966 2 4 5 1
	2147			307 3.567 307 7586	2.422 10951	58.485 7874	1.000 69.51 -6970 -2008 3245
	2148			307 5.489	1.937	59.600	
ANISOU	2148		ARG	307 10714	8150	3930	-5986 -3291 2028
ATOM ANISOU	2149 2149		THR THR	308 10.347 308 2759	2.147 2587	54.048 3364	
ATOM	2150		THR	308 2739	1.009	53.794	
ANISOU	2150		THR	308 3382	2649	3268	-360 52 1 5 0
ATOM ANISOU	<ul><li>2151</li><li>2151</li></ul>		THR	308 10.602		54.382	
ATOM	2152	0	THR THR	308 5251 308 10.610	2520 -1.292	4044	-768 16279 1.00031.44
ANISOU		Ö	THR	308 4573	2676	4696	-457 -1745 <b>-</b> 4 0
ATOM		CB	THR	308 12.615	1.279		1.000 23.51
ANISOU ATOM	<ul><li>2153</li><li>2154</li></ul>		THR THR	308 3718 308 13.195	2086	3131	413 -694 5 4 2
				308 2711	2.410 2503	53.705 3754	1.000 23.61 153 437 - 9
ATOM	2155		THR	308 13.573	0.141	54.117	
ANISOU	2155			308 4427	2796	2796	927 -329 - 18
ATOM ANISOU	2156 2156		SER SER	309 10.066 309 3759	-0.156 2774	55.596 4252	1.000 28.39 -19
ATOM	2157		SER	309 9.488		56.238	
ANISOU	2157		SER	309 6110	3146	3925	-1066 -1089 1626
ATOM ANISOU	2158 2158		SER SER	309 8.109		55.724	
ATOM	2159	0	SER	309 6442 309 7.672	3910 -2.884	5383 55.952	
ANISOU		-	SER	309 11389	5141	5146	
ATOM			SER	309 9.450			1.000 31.61
ANISOU ATOM	2160		SER SER	309 4863		4188	-483 368 962 1.00038.99
ANISOU			SER	309 4731			313 -2249 - 496
ATOM	2162	N	LYS	310 7.391	-0.868	55.032	
ANISOU				310 5502			-539 -1369 1583
ATOM ANISOU			IUM IUM	312 8.574 312 1690			1.000 11.05 -101 -237 7 1
ATOM	2164		AKG	313 5.987			1.000 19.65
ANISOU			AKG	313 2777	2119	2572	258 -117 5 5 6
ATOM ANISOU	2165		AKG	313 4.799			1.000 20.82
ATOM	2165		AKG AKG	313 2957 313 6 643			514 -234264 $1.00017.79$
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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	21222222222222222222222222222222222222	225553445553344 1234888888888888888888888888888888888888	AKKGGGGGGGGGG4444HHHHHHHHHHHHHHHHHHHHHHH	33333333333333344444555555555555555555	-6.873 10.676 -0.077 5.761 29.132 10.871 26.965 23.353 21.429 9.122 27.843 -14.415 15.253 14.080 17.770 3.671 -15.686 10.165 23.736 -1.386 -1.386 -1.	19.199 24.642 -4.179 21.786 13.656 31.449 32.371 24.457 29.1063 11.567 17.352 20.056 31.482 21.673 21.657 21.657	43.074 52.602 47.100 46.406 40.872 46.041 51.741 52.741 51.741 53.329 53.329 53.431 51.702 53.536	1.000 16.38 1.000 20.55 1.000 27.41 1.000 15.22 1.000 17.40 1.000 18.40 1.000 16.70 1.000 18.71 1.000 18.96 1.000 20.41 1.000 18.39 1.000 24.87 1.000 27.76 1.000 27.76 1.000 27.76 1.000 27.58 1.000 27.58 1.000 27.58 1.000 27.56 1.000 28.33 1.000 28.33 1.000 28.33 1.000 29.36 1.000 24.02 1.000 21.62 1.000 31.65 1.000 19.59
				526				
MOTA	2205	WO						
				528	23.736			
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	2210		HOH	531	0.980	35.65/		
ATOM	2211		НОН	533	-12.450	16.848		1.000 30.57
	2212	OW	НОН		-9.418	16.139		1.000 28.42
	2213		НОН	535	32.711			1.000 31.44
ATOM ATOM	<ul><li>2214</li><li>2215</li></ul>		HOH		27.068	24.587	55.468	1.000 23.32
	2215		HOH HOH			11.832		1.000 10.73
ATOM	2217		НОН		0.922	16.158 2.590	35.074 35.058	1.000 12.26 1.000 14.79
MOTA	2218	OW	нон			3.709		1.000 14.79
MOTA	2219	OW	НОН		11.711	16.898	30.416	

- 162 -

2220 OW ATOM 542 15.389 11.536 32.065 HOH 1.000 17.88 2221 OW 6.995 1.000 17.47 ATOM HOH 543 18.496 52.191 2222 OW ATOM 544 19.848 HOH 22.580 35.334 1.000 17.28 2223 OW ATOM 545 ~0.387 4.787 41.967 HOH 1.000 13.22 2224 OW 12.662 ATOM HOH 546 23.502 35.308 1.000 18.14 2225 OW ATOM 25.236 HOH 547 10.332 33.926 1.000 19.05 2226 OW 34.090 ATOM HOH 548 21.447 20.605 1.000 17.24 2227 OW ATOM HOH 549 8.164 7.685 27.077 1.000 25.40 2228 OW 550 14.393 40.321 ATOM HOH -5.127 1.000 15.88 551 12.873 2229 OW 29.356 ATOM HOH 39.662 1.000 16.45 2230 OW ATOM HOH 552 11.974 58.426 24.144 1.000 19.71 2231 OW HOH 553 17.521 7.949 33.182 1.000 17.90 ATOM 2232 OW HOH 43.340 ATOM 554 3.401 2.691 1.000 23.76 2233 OW 1.000 18.44 ATOM HOH 555 18.669 28.057 40.079 2234 OW 30.017 HOH 556 10.827 12.928 ATOM 1.000 19.57 2235 OW 66.466 ATOM 16.270 557 20.630 1.000 20.84 HOH 2236 OW ATOM HOH 558 11.315 20.266 64.044 1.000 21.62 2237 OW 559 26.277 14.516 1.000 16.22 ATOM HOH 43.946 ATOM 2238 OW HOH 560 9.616 15.488 32.365 1.000 19.40 2239 OW 1.000 22.74 ATOM HOH 561 8.888 4.903 27.857 ATOM 2240 OW HOH 562 20.496 -1.851 42.511 1.000 22.98 2241 OW 1.000 26.36 ATOM HOH 563 17.033 29.415 38.332 2242 OW HOH 564 18.595 6.141 37.697 ATOM 1.000 25.10 2243 OW MOTA 565 22.446 13.893 31.420 1.000 29.00 HOH 2244 OW ATOM HOH 566 6.586 3.577 28.350 1.000 27.82 2245 OW ATOM HOH 567 6.250 20.077 30.961 1.000 23.27 ATOM 2246 OW 568 7.341 HOH 16.113 31.186 1.000 28.59 ATOM 2247 HOH OW 569 16.090 32.070 42.552 1.000 33.08 2248 OW HOH 570 11.500 28.806 37.258 1.000 25.17 ATOM 1.000 28.58 ATOM 2249 OW HOH 571 12.901 58.591 26.768 2250 OW HOH ATOM 572 -17.071 17.043 50.450 1.000 28.82 2251 OW ATOM 7.705 1.000 3.9.05 HOH 573 25.262 37.199 2252 OW 51.734 ATOM 574 32.884 26.440 HOH 1.000 29.03 2253 OW 575 -1.199 1.000 14.86 ATOM HOH 19.088 42.527 2254 OW ATOM 576 - 4.38933.026 63.392 1.000 29.56 HOH 2255 OW 32.249 ATOM 577 17.569 25.732 1.000 20.62 HOH 2256 578 -19.107 12.822 67.516 ATOM HOH OW 1.000 22.35 19.198 2257 OW 51.975 1.000 22.51 HOH 579 29.333 ATOM 2258 OW ATOM HOH 27.635 51.903 580 27.950 1.000 25.40 2259 OW 581 -21.085 14.501 68.535 ATOM HOH 1.000 21.19 2260 OW ATOM HOH 582 1.529 17.378 33.953 1.000 25.29 ATOM 2261 OW 583 9.138 HOH 20.887 66.894 1.000 33.92 ATOM 2262 OW 584 -11.896 19.091 HOH 44.780 1.000 17.48 ATOM 2263 OW HOH 585 6.382 12.597 43.347 1.000 22.09 2264 OW ATOM HOH 586 17.762 21.268 29.046 1.000 20.79 ATOM 2265 OW HOH 587 -11.500 25.438 41.729 1.000 29.68 ATOM 2266 OW 588 7.877 1.046 29.689 1.000 27.70 HOH 589 27.985 MOTA 2267 OW HOH 13.540 42.235 1.000 25.91 MOTA 2268 OW HOH 590 1.276 14.852 34.021 1.000 20.41 MOTA 2269 OW HOH 591 24.622 24.179 41.242 1.000 26.77 2270 OW ATOM 14.096 36.006 1.000 27.92 592 0.404 HOH 36.981 57.827 1.000 31.86 ATOM 2271 OW HOH 593 -2.835 2272 OW ATOM HOH 594 3.276 0.788 39.940 1.000 32.07 ATOM 2273 OW HOH 595 11.025 -8.794 31.468 1.000 27.18 ATOM 2274 OW HOH 2.276 42.639 1.000 29.74 596 6.301 ATOM 2275 OW HOH 597 29.302 16.146 62.924 1.000 43.75 2276 OW ATOM HOH 20.964 67.011 598 19.039 1.000 30.85 ATOM 2277 OW HOH 22.088 64.518 1.000 42.62 599 8.380 ATOM 2278 OW 600 21.480 10.826 34.742 1.000 25.74 HOH ATOM 601 -2.907 21.956 38.566 1.000 30.92 2279 OW HOHHOH 602 -3.928 ATOM 2280 OW 29.841 43.352 1.000 43.96

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- 163 -2281 OW ATOM 603 2.885 HOH 21.563 34.437 1.000 33.10 ATOM 2282 OW HOH 604 11.801 6.043 25.270 1.000 38.18 2283 OW ATOM 605 -1.019 HOH 17.197 40.472 1.000 18.48 ATOM 2284 OW HOH 23.349 606 18.382 68.110 1.000 22.54 2285 OW ATOM HOH 607 - 8.1418.137 45.609 1.000 17.64 ATOM 2286 OW 608 5.022 HOH 2.667 51.700 1.000 24.29 ATOM 2287 OW HOH 609 17.557 33.490 10.755 1.000 21.94 2288 OW ATOM HOH 610 11.222 1.201 49.675 1.000 20.61 ATOM 2289 OW HOH 35.047 611 4.243 50.509 1.000 22.18 2290 OW ATOM 612 11.103 HOH 4.031 56.082 1.000 22.08 2291 OW MOTA HOH 613 11.366 31.522 36.791 1.000 32.32 2292 OW ATOM 614 -21.189 24.787 HOH 52.739 1.000 31.83 2293 OW MOTA 615 7.847 HOH -1.491 30.674 1.000 24.77 MOTA 2294 OW 616 19.041 HOH 11.937 31.445 1.000 25.97 2295 OW ATOM HOH 29.879 617 6.221 40.410 1.000 29.24 ATOM 2296 OW HOH 618 17.266 5.933 35.280 1.000 23.72 ATOM 2297 OW HOH 619 5.983 -7.21528.510 1.000 28.19 ATOM 2298 OW 620 22.574 HOH 8.129 57.639 1.000 30.97 2299 OW MOTA 621 2.553 HOH 7.806 60.287 1.000 28.77 MOTA 2300 OW 622 29.939 HOH 25.812 51.234 1.000 34.00 ATOM 2301 OW 623 2.205 HOH 34.823 53.632 1.000 25.88 ATOM 2302 OW HOH 624 18.091 13.838 67.343 1.000 28.46 ATOM2303 OW HOH 625 8.342 3.195 58.475 1.000 26.84 ATOM 2304 OW HOH 626 -16.086 18.427 42.790 1.000 31.11 MOTA 2305 OW HOH 627 -2.098 13.445 35.620 1.000 27.48 ATOM 2306 OW 628 0.481 HOH 30.471 42.834 1.000 32.55 ATOM 2307 OW 629 13.368 HOH 33.845 42.899 1.000 28.70 ATOM 2308 OW 630.-13.792 14.642 HOH 51.533 1.000 25.58 2309 OW MOTA HOH 631~3.299 1.461 29.242 1.000 39.62 2310 OW ATOM 632 -16.012 20.690 HOH 46.705 1.000 27.75 ATOM 2311 OW HOH 633 19.606 8.142 31.259 1.000 27.02 ATOM 2312 OW 634 5.077 HOH 57.205 7.954 1.000 30.59 ATOM 2313 OW 635 -1.502 6.963 HOH 45.877 1.000 35.68 ATOM 2314 OW HOH 636 9.974 17.449 38.804 1.000 21.84 ATOM 2315 OW 637 -22.829 12.836 HOH 67.228 1.000 25.04 2316 OW ATOM HOH 638 6.275 34.333 39.722 1.000 25.88 ATOM 2317 OW HOH 639 2.248 19.798 56.051 1.000 26.67 ATOM 2318 OW 640 -20.552 17.013 HOH 67.454 1.000 31.34 2319 OW ATOM HOH 641 9.298 16.570 28.911 1.000 29.96 2320 OW ATOM 642 - 1.732HOH 11.113 1.000 28.13 60.074 2321 OW ATOM HOH 643 34.157 23.604 44.657 1.000 36.36 2322 OW ATOM HOH 644 24.298 20.199 33.576 1.000 34.90 ATOM 2323 OW HOH 645 13.803 -4.667 31.570 1.000 32.66 ATOM 2324 OW 646 6.295 HOH -2.59429.009 1.000 34.61 ATOM 2325 OW HOH 647 5.623 37.039 1.000 28.08 49.318 ATOM 2326 OW 648 -18.805 19.286 HOH 46.868 1.000 38.32 ATOM 2327 OW 649 16.026 35.829 HOH 49.382 1.000 34.45 ATOM 2328 OW 650 -12.187 28.769 HOH 45.330 1.000 27.36 2329 OW ATOM HOH 651 21.344 5.778 55.101 1.000 27,43 ATOM 2330 OW HOH 652 -1.848 2.125 32.240 1.000 32.02 ATOM 2331 OW HOH 653 -14.568 18.811 1.000 29.95 55.775 2332 OW ATOM HOH 654 -8.655 26.254 38.301 1.000 32.07 ATOM 2333 OW 655 18.836 HOH 13.542 1.000 32.24 28.102 2334 OW ATOM НОН 656 16.217 14.669 25.619 1.000 33.35 MOTA 2335 OW HOH 657 28.678 14.477 38.043 1.000 30.94 ATOM 2336 OW 658 -11.834 15.408 HOH 1.000 33.25 53.330 ATOM 2337 OW HOH 659 -1.317 38.273 59.599 1.000 34.45 ATOM 2338 OW HOH 660 8.784 13.918 28.681 1.000 33.62 ATOM 2339 OW HOH 661 -3.058 14.508 47.405 1.000 28.79 ATOM 2340 OW 662 10.968 HOH 33.651 1.000 36.21 38.533 ATOM

21.602

53.665

1.000 29.25

663 28.960

2341 OW

HOH

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ATOM	2342 OW	нон	661 -	10.709	26.808	39.175	1.000 42.71
ATOM	2342 OW	HOH		7.790	7.093	55.023	1.000 30.29
ATOM	2343 OW 2344 OW						
		HOH		1.404	24.865	29.848	1.000 34.55
ATOM	2345 OW	НОН		15.418	19.777	58.341	1.000 33.82
ATOM	2346 OW	нон		.000	0.000	37.259	0.330 49.90
ATOM	2347 OW	нон		9.652	24.610	33.660	1.000 31.77
ATOM	2348 OW	НОН		7.188	9.619	29.950	1.000 29.94
ATOM	2349 OW	НОН		7.708	2.958	28.338	1.000 34.94
ATOM	2350 OW	HOH		0.059	3.652	30.079	1.000 32.23
ATOM	2351_OW	HOH	673 2	9.037	20.923	56.153	1.000 28.52
ATOM	2352 OW	HOH	674 -	15.435	31.088	53.795	1.000 35.61
ATOM	2353 OW	HOH	675 -	12.846	21.220	61.856	1.000 38.79
ATOM	2354 OW	HOH	676 1	.0.299	39.666	49.554	1.000 40.30
ATOM	2355 OW	HOH	677 -	5.921	28.822	41.521	1.000 34.01
ATOM	2356 OW	HOH	678 6	.029	39.991	46.094	1.000 42.69
ATOM	2357 OW	HOH	679 3	5.052	23.156	52.356	1.000 40.17
ATOM	2358 OW	HOH		12.008	38.355	51.601	1.000 35.18
ATOM	2359 OW	HOH	681 3	.061	13.047	53.152	1.000 35.17
ATOM	2360 OW	НОН	682 1	379	2.075	27.532	1.000 46.38
ATOM	2361 OW	HOH	683 -	0.516	-2.480	37.686	1.000 21.77
ATOM	2362 OW	HOH	684 4	1.567	10.310	43.503	1.000 24.86
MOTA	2363 OW	НОН		9.443	5.558	61.133	1.000 36.06
ATOM	2364 OW	нон		3.205	29.499	40.656	1.000 36.99
MOTA	2365 OW	нон		32.498	16.774	43.447	1.000 41.18
	2366 OW				_		1.000 35.56
	2367 OW	НОН					1.000 30.05
ATOM	2368 OW	HOH					1.000 32.51
	2369 OW	НОН					1.000 33.34
ATOM	2370 OW	НОН	-				1.000 34.99
ATOM	2371 OW						1.000 39.38

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#### **CLAIMS**

- Deacetoxycephalosporin C synthase (DAOCS) having a structure designated by the X-ray co-ordinates of structure A or structure B herein.
- DAOCS in the form of a complex with a metal, e.g. iron or lead, and optionally in the presence of a substrate and/or a substrate analogue or inhibitor, having a structure designated by the X-ray co-ordinates herein.
- DAOCS as claimed in claim 2, wherein the substrate is penicillin N, penicillin G, 2-oxoglutarate or dioxygen, and the inhibitor is selected from N-oxalylamino acids, pyridine-carboxylates and nitrous oxide.
- 4. Use of the three-dimensional structure of DAOCS for the modification of DAOCS or other related 2-oxoglutarate dependent enzyme.
  - Use as claimed in claim 4, wherein the related 2-oxoglutarate dependent enzyme is DACS, DAOC/DACS or the oxygenase enzyme involved in the introduction of the  $7\alpha$ -methoxy group into cephamycin C.
  - 6. Use as claimed in claim 5 for the modification of DAOCS, DACS or DAOC/DACS such that they accept unnatural substrates more efficiently than the wild type enzymes.

Use as claimed in claim 5 for the modification of DAOCS, DAOC/DACS such that they convert natural substrates to pharmaceuticals or useful intermediates in the preparation of pharmaceuticals.

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Use as claimed in claim 6 wherein the unnatural substrates are penicillins including penicillin G, penicillin V, 6-aminopenicillanic acid, amoxycillin, or penicillins with a phenyl glycine or p-hydroxyphenyl glycine side chain.

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9. Use as claimed in claim 6 wherein the unnatural substrate is a cephalosporin.

10. Use as claimed in claim 6 wherein the unnatural substrate is an amino acid, including the proteinogenic amino acids, or a peptide.

11. Use as claimed in any one of claims 6-8, wherein penicillin G, penicillin V, another unnatural substrate or penicillin N is converted to a cephalosporin or exomethylene cephalosporin.

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12. An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted:

Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

An enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in

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one of the above.

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- An enzyme according to claim 12 or claim 13 which is a mutant of DAOCS or DACS or DAOC/DACS.
- An enzyme as claimed in any one of claims 12-14, wherein both the side chain and the penicillin/cephalosporin binding sites of penicillin N or DAOC are modified and at least one of the residues specified in claims 12 and 13 is changed or deleted.
- 16. An enzyme as claimed in any one of claims 12-15, wherein two or more complementary mutations are introduced to create or delete a binding interaction, including H-bonds, electrostatic, or hydrophobic interactions.
  - 17. A gene encoding for the enzyme of any one of claims 12-16.

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- A micro-organism capable of expressing the gene of claim 17 under fermentation conditions.
- 19. Use of micro-organisms of claim 18 for the production of beta-lactams of the penicillin or cephalosporin (including cepham) families.

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- 20. Use as claimed in claim 19 wherein the micro-organism contains another modified enzyme of the penicillin and cephalosporin biosynthesis pathway including isopenicillin N synthase, amidohydrolase/acetyltransferase, or L-delta-(aminoadipoyl)-L-cysteine-D-valine (ACV) synthetase.
- 21. A method which comprises using the three-dimensional structure of DAOCS for determining or predicting the structure of another related 2-oxoglutarate dependent enzyme or related enzyme not from the penicillin and cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the other enzyme or for designing an inhibitor for the other enzyme.
- 22. A method as claimed in claim 21 wherein the said other
  related 2-oxoglutarate dependent enzyme or related enzyme is
  1-aminocylopropane-1-carboxylate oxidase, gibberellin C-20 oxidase,
  flavone synthase, flavanone 3β-hydroxylase, hyoscyamine 6β-hydroxylase,
  prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, lysyl
  hydroxylase, proline hydroxylases, γ-butyrobetaine hydroxylase, enzymes
  in herbicide resistance mechanisms, clavaminate synthase, an oxygenase
  enzyme involved in the biosynthesis of carbapenems, the so called
  ethylene forming enzyme from *Pseudomonas syringe*,
  p-hydroxyphenylpyruvate dioxygenase, and an oxygenase enzyme
  involved in the oxidation of phytol in human liver peroxisomes.

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23. A method as claimed in claim 21 or 22, wherein the said other enzyme is modified, by deletion or addition or alteration; at one or more of the sites defined in claim 12 or claim 13; or using the following information for the design or an inhibitor: Asp185, His183 and His243 act as ligands to the iron; Arg258 and Ser260 and the Fe bind the

2-oxoglutarate; Met180, Phe225, Leu31 and Val245 are close to the iron binding site; Tyr33, Arg160, Arg162, Phe164, Ile192, Gln194, Leu204, Leu223, Leu215 are important for the construction of the part of the active site binding 2-oxoglutarate; and Arg160 and Arg162 are important for binding an amino acid or peptide derived substrate.

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- A method as claimed in any one of claims 21-23, wherein the said other enzyme is prolyl 4-hydroxylase, prolyl 3-hydroxylase, aspartyl hydroxylase, or lysyl hydroxylase and the inhibitor is to be used for the treatment of human diseases including fibrotic diseases including liver cirrhosis and arthritis.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is p-hydroxyphenylpyruvate dioxygenase and the inhibitor is to be used in the treatment of certain genetic disorders.
- A method as claimed in any one of claims 21-23, wherein the said other enzyme is involved in herbicide resistance and the information is to be used to design new herbicides to overcome the problem of resistance.

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SUBSTITUTE SHEET (RULE 26)

# INTERNATIONAL SEARCH REPORT

Inte. .ional Application No PCT/GB 98/03860

A. CLASSII IPC 6	FICATION OF SUBJECT MATTER C12N15/52 C12N9/00 C12P35/0	0 \	
	International Patent Classification (IPC) or to both national classifica	ition and IPC	
B. FIELDS  Minimum do	cumentation searched (classification system followed by classification	on symbols)	<del></del>
IPC 6	C12N C12P	<u>-</u>	
Documentat	ion searched other than minimum documentation to the extent that so	uch documents are included in the fields sea	arched
Electronic d	ata base consulted during the international search (name of data bas	se and, where practical, search terms used)	
	ENTS CONSIDERED TO BE RELEVANT		Calana at the state of
Category 3	Citation of document, with indication, where appropriate, of the rele	evant passages	Relevant to claim No.
X	CORTES, JESUS ET AL: "Purificati characterization of a 2-oxoglutarate-linked ATP-independence of the control of	ident	1
	deacetoxycephalosporin C synthase Streptomyces lactamdurans"	. 01	
	J. GEN. MICROBIOL. (1987), 133(11	.),	
	3165-74 CODEN: JGMIAN; ISSN: 0022-	-1287,	
<b>~</b>	1987, XP000035085 see the whole document		2 3
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X Furt	her documents are listed in the continuation of box C.	χ Patent family members are listed	in annex.
° Special ca	ategories of cited documents :	"T" later document published after the inte	mational filing date
	ent defining the general state of the art which is not	or priority date and not in conflict with cited to understand the principle or the	the application but
"E" earlier	dered to be of particular relevance document but published on or after the international	invention "X" document of particular relevance; the o	claimed invention
filing of "L" docume	date  ent which may throw doubts on priority claim(s) or	cannot be considered novel or cannot involve an inventive step when the do	be considered to
which	is cited to establish the publication date of another n or other special reason (as specified)	"Y" document of particular relevance; the cannot be considered to involve an in-	laimed invention
"O" docum	ent referring to an oral disclosure, use, exhibition or means	document is combined with one or moments, such combination being obvious	ore other such docu-
"P" docum	ent published prior to the international filing date but	in the art.	·
	actual completion of the international search	"&" document member of the same patent  Date of mailing of the international sea	
	.5 March 1999	26/03/1999	
Name and	mailing address of the ISA	Authorized officer	
	European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk		
	Tel. (+31-70) 340-2040, Tx. 31 651 epo ni, Fax: (+31-70) 340-3016	Hix, R	

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## INTERNATIONAL SEARCH REPORT

Int. cional Application No PCT/GB 98/03860

C/Contine	ration) DOCUMENTS CONSIDERED TO BE RELEVANT	PCT/GB 98/03860
Category '		Relevant to claim No.
<b>X</b>	ROLLINS, M. J. ET AL: "Purification and initial characterization of deacetoxycephalosporin C synthase from Streptomyces clavuligerus" CAN. J. MICROBIOL. (1988), 34(11), 1196-202 CODEN: CJMIAZ; ISSN: 0008-4166,	
Y	1988, XP002095821 see the whole document	2,3, 21-26
X	ROLLINS M J ET AL: "ISOPENICILLIN N SYNTHASE AND DEACETOXYCEPHALOSPORIN C SYNTHASE ACTIVITIES DURING DEFINED MEDIUM FERMENTATIONS OF STREPTOMYCES-CLAVULIGERUS EFFECT OF OXYGEN AND IRON SUPPLEMENTS" CAN J MICROBIOL, (1989) 35 (12), 1111-1117. CODEN: CJMIAZ. ISSN:	
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X	DOTZLAF, JOE E. ET AL: "Purification and properties of deacetoxycephalosporin C synthase from recombinant Escherichia coli and its comparison wit the native enzyme purified from Streptomyces clavuligerus" J. BIOL. CHEM. (1989), 264(17), 10219-27 CODEN: JBCHA3; ISSN: 0021-9258, 1989, XP002095823	. 1
Y	see the whole document	2,3, 21-26
<b>X</b>	BALDWIN J E ET AL: "HIGH-LEVEL SOLUBLE EXPRESSION AND PURIFICATION OF DEACETOXYCEPHALOSPORIN C-DEACETYLCEPHALOSPORIN C SYNTHASE." BIOORG MED CHEM LETT, (1992) 2 (7), 663-668. CODEN: BMCLE8. ISSN: 0960-894X., XP002095824	1
1	see the whole document	2,3, 21-26
<b>(</b>	EP 0 366 354 A (LILLY CO ELI) 2 May 1990 see the whole document	1 2,3, 21-26
<b>(</b>	BALDWIN J E ET AL: "HIGH-LEVEL SOLUBLE EXPRESSION AND PURIFICATION OF DEACETOXYCEPHALOSPORIN C-DEACETYLCEPHALOSPORIN C SYNTHASE." BIOORG MED CHEM LETT, (1992) 2 (7), 663-668. CODEN: BMCLE8. ISSN: 0960-894X., XP002095825	
<b>(</b>	see the whole document	2,3, 21-26

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### IN RNATIONAL SEARCH REPORT

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